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The time-independent Schrödinger equation in the frame of Feynman's version of quantum mechanics

Jozef Hanc[a]

Institute of Physics, Faculty of Science, P.J. Safarik University

Park Angelinum 9, 040 01 Kosice, Slovakia

One of the weaknesses of the Feynman's path integral approach is primarily mathematically complicated finding of eigenvalues and eigenstates, which are "easily obtainable" from the Schrödinger equation. We have developed and started testing a new heuristic derivation of time-independent Schrödinger equation in terms of Feynman's approach. With the help of this derivation students through spreadsheets in Excel or JAVA applets can model and find naturally and simply eigenwavefunctions and energy eigenvalues for any one-dimensional potential. A very significant advantage of this new approach consists in the use of high school elementary vector algebra and the Pythagorean Theorem only, so there is no explicit use of operators, partial derivatives or differential equations. The procedure and developed teaching materials, providing deep conceptual understanding of eigenstates and energy quantization, are most suitable for algebra based introductory physics courses, quantum mechanics introductions for future high school physics teachers, engineers, chemists or biologists. With small changes the derivation is also applicable and very useful in traditional quantum mechanics courses starting from Schrödinger formulation.

I. PREVIEW: SEVERAL WORDS ABOUT MOTIVATION FOR THE PAPER

In this section I would like to introduce reasons, which motivated me for this paper. (1) *The first reason of my motivation is my personal interest in teaching and study of Feynman's quantum mechanics* (basic ideas and our results are in the Berlin MPTL 10 contribution [3]). If I summarize my activities dealing with Feynman's quantum mechanics, this year (2006) is 8th year of my study and pedagogical research dealing with Feynman's version of quantum theory; 6th year of my teaching this approach; 1th year after finishing my external Ph.D. study with thesis entitled: *Feynman's approach in teaching quantum mechanics.*

Three important events led to my conversion to the Feynman approach in teaching quantum theory. As 18 years old in 1992 I was gifted by three volumes (five in Slovak version) of famous Feynman's lectures on physics and during my university study Richard Feynman became my greatest hero of science, man of legendary proportions among physicists.

In 1998 I obtained Feynman's popular QED book: *The Strange Theory of Light and Matter* [2]. This book, collections of public lectures about quantum electrodynamics and basic ideas of Feynman's many paths approach was absolutely great and fascinating for me. So during May of 1998 I translated it into Slovak with my friend and colleague Slavo Tuleja. Later this translation officially appeared in Slovakia in 2000.

The third event leading to my conversion was reading Edwin Taylor's Oersted medal speech in American Journal of Physics [8]. I was really impressed by the following Edwin Taylor's words: *„One day several years ago it dawned on me that the electron is stupid. Or - so as not to insult any of God's creatures - let us say that the electron is brainless; no one can argue with that! ... The brainless electron has no chance whatsoever to decode the mysteries of the Schrödinger equation. It requires a simpler set of instructions... Feynman stands astride the Universe and issues a three-word command so simple that every particle can obey:* ***Explore all paths!*** *Particles are so brainless that they cannot choose a single path, so explore them all. And from this blind exploration come the essential surprises, paradoxes, strangeness - and power! - of quantum mechanics."*

[a]email: jozef.hanc@upjs.sk

(2) The second reason for this contribution, also personal, was an interesting discussion after my MPTL 10 workshop lecture with one of participants whose objections were following:

- *Be careful* in using ideas from public lectures like Feynman's QED. Created ideas in minds of students and ordinary people after any public lecture are usually so wrong that it causes complete misunderstanding of physics and real world around us.
- *Try to avoid* confusing audience, if you compare student's understanding quantum mechanics from courses based on two different versions (Schrödinger and Feynman).

In response to the first criticism I use my experience showing that this should not be our case. Results of testing and assigning demonstrate that students of our courses have much better conceptual understanding, intuitive feel and skills to describe and predict quantum behavior in comparison with students of traditional courses. They are better in both cases: time-dependent and time-independent situations. In addition our approach leads to more considerable student's enthusiasm.

Concerning the second objection it consists in the fact that Schrödinger's wave mechanics is easy and very good for describing time-independent states – eigenfunctions, one of most important part of any university quantum course whereas Feynman's approach is much more difficult in doing these descriptions and it is especially not very suitable in finding stationary states. However as it will be seen bellow the opposite is true. In our pedagogical approach describing stationary states in the frame of Feynman's quantum mechanics is less abstract, mathematically much simpler and physically more understandable.

(3) The third motivating historical reason for this paper was important date of this year, *13 March 2006*. This date marks the 80th anniversary of the official the time-independent Schrödinger equation birth. On this day 80 years ago the Schrödinger paper *Quantization as a Problem of Eigenvalues (Part I)* with the time-independent Schrödinger equation appeared in issue 4 of Annalen der Physik [6]. In the following months Schrödinger published other five excellent articles, which together with the first mentioned we understand as the starting point and the rise of wave mechanics [4].

Erwin Schrödinger

(4) The last motivation is the meaning of the Schrödinger's equation, the most quoted equation in the scientific literature of the twentieth century [4]. The Schrödinger equation is the cornerstone of the wave mechanics – traditional approach dominating at least last 50 years in introductory quantum mechanics courses. The time-independent Schrödinger equation, which we call for rest of the paper only the Schrödinger equation or shortly the SchE:

$$-\frac{\hbar^2}{2m}\frac{\mathrm{d}^2\psi(x)}{\mathrm{d}x^2}+V\psi(x)=E\psi(x) \qquad (1)$$

provides a general method:

- determining wavefunctions representing time independent stationary states, called the energy eigenfunctions.
- finding corresponding energy levels, eigenvalues.

For modeling purposes we can rewrite Eq. (1) into the simplest numerical version of the SchE. If we divide the x axis into many equally spaced discrete points and use one of definitions of the second derivative:

$$\frac{\mathrm{d}^2\psi(x)}{\mathrm{d}x^2}=\lim_{\Delta x\to 0}\frac{\psi(x+\Delta x)-2\psi(x)+\psi(x-\Delta x)}{\Delta x^2}$$

we get its finite-difference approximation:

$$\frac{\mathrm{d}^2\psi(x)}{\mathrm{d}x^2} \approx \frac{\psi(x+\Delta x)-2\psi(x)+\psi(x-\Delta x)}{\Delta x^2}$$

leading to a numerical version of the SchE:

$$\psi(x+\Delta x)=2\psi(x)-\psi(x-\Delta x)-\frac{2m\Delta x^2}{\hbar^2}[E-V(x)]\psi(x) \qquad (2)$$

used and appropriate for modeling in introductory quantum mechanics courses.

II. MAKING A MODEL FOR STATIONARY STATES: HEURISTIC DERIVATION OF THE SCHRÖDINGER EQUATION.

Let's go pay attention to basic steps of a teaching material in our quantum mechanics course. The pedagogical query is how students make a model for stationary states or in other words how they heuristically discover the Schrödinger equation (2) in terms of Feynman's approach.

Initial knowledge of students

Student's starting knowledge before finding the model (the SchE) is:

- fundamental principles of Feynman's approach (see e. g. [7], [2] or [3])
- approximations of sin and cos functions; there is an elementary geometrical high school argument based on the Phytagorean Theorem proving that for small angle ε $\sin\varepsilon \approx \varepsilon$, $\cos\varepsilon \approx 1-\varepsilon^2/2$.
- shape of the wavefunction at some fixed moment *t* of particles emitted from a source of a completely coherent character with very precise emission energy *E*. This wavefunction is known for students from one of our previous tutorials as a result of fundamental principles and it is a set of quantum arrows – one for each discrete point along *x* axis – satisfying conditions described by fig.1.

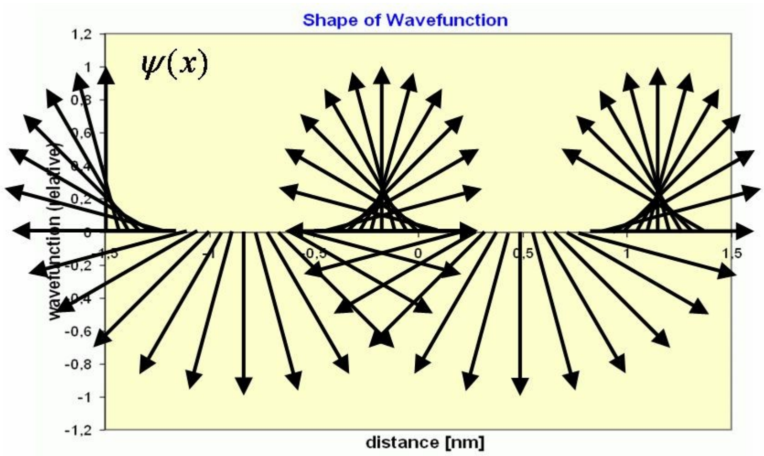

Fig. 1: *The vawefunction of particles emitted from a coherent source with energy E. Each arrow $\psi(x)$ according to the fundamental principles represents an arrow for outcome - finding emitted particle at given place whereas square of the arrow's length is probability of this outcome. In addition any arrow makes extra number of rotations with respect to quantum arrow of the source given by the expression:* $\begin{pmatrix}\text{number of}\\ \text{rotations}\end{pmatrix}=\frac{1}{h}\,p\cdot\begin{pmatrix}\text{distance}\\ \text{from the source}\end{pmatrix}$ *, where $2mE=p^2$ and h is the Planck constant.*

If students explore wavefunction faraway from the source, the wavefunction is their first example of stationary state wavefunction. In this wavefunction students can recognize a repeating pattern. Particularly after a certain distance the direction of arrows repeats. What is this distance? Using the expression for rotations of arrows: $(\text{number of rotations})=\frac{1}{h}p\cdot x$, we can find that mentioned distance for one turn of the arrow along x axis has to satisfy a condition:

$$1=\begin{pmatrix}\text{one}\\ \text{turn}\end{pmatrix}=\frac{1}{h}p\cdot\begin{pmatrix}\text{distance}\\ \text{for one turn}\end{pmatrix} \qquad (3)$$

Such behavior is similar to behavior of waves. And Eq. (3) is nothing else as a restatement of the well-known de Broglie relation $\lambda=h/p$, where de Broglie wavelength λ is just the distance for one arrow's turn along space and p is connected to energy of particles by expression $p^2=2mE$.

Local description of the de Broglie wave

To make next step to the required Schrödinger equation (2), students also find a local description of the de Broglie wave – the equation describing behavior of wave function arrows in a small region at any place. Such situation in vicinity of some specific point x is depicted in fig.2 .

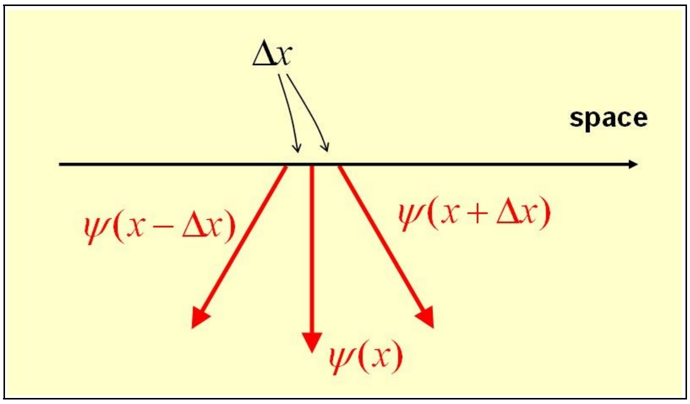

Fig. 2

If we put tails of these three arrows to one common point, then from the previous global description of the de Broglie wave we know that angles between arrows whose tails are equally spaced through Δx must be the same and equal to $\varepsilon=2\pi(p/h)\Delta x=(p/\hbar)\Delta x$. Since Δx is taken very small, angle Δx is also small. The arrows geometrically form a parallelogram of which one diagonal includes the middle arrow $\psi(x)$ and the second diagonal is perpendicular with it as it is shown in Fig. 3.

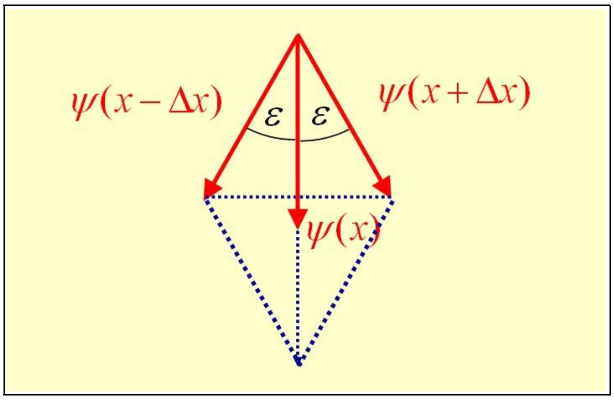

Fig . 3

This situation is only possible if vector average of outer arrows is scalar multiple of the middle arrow and from the formed right triangles we see the constant of this multiplication is nothing else as cosine of angle ε :

$$\frac{\psi(x+\Delta x)-\psi(x-\Delta x)}{2}=\psi(x)\cos\varepsilon$$

Since angle ε is very small, it is time to apply small angle approximations of cosine which yields the equation:

$$\frac{\psi(x+\Delta x)-\psi(x-\Delta x)}{2}=\psi(x)\left(1-\frac{\varepsilon^2}{2}\right), \text{ where } \varepsilon^2=\left(\frac{p}{\hbar}\right)^2\Delta x^2=\frac{2mE\Delta x^2}{\hbar^2}.$$

After two simple arrangements (multiplication and subtraction) of both sides of the last equation, we get a numerical version of the SchE for free particles:

$$\psi(x+\Delta x)=2\psi(x)-\psi(x-\Delta x)-\frac{2m\Delta x^2}{\hbar^2}E\,\psi(x) \qquad (4)$$

This equation expresses simultaneously the condition of stationarity of the free particle's wavefunction.

Generalization to varying potential energy

Now we can make heuristic generalization for case with arbitrary reasonable physical potential energy function $V(x)$. In any small region around a given point x the potential energy $V(x)$ is practically constant and we could consider the particle as a free particle with kinetic energy $E-V(x)=p^2/2m$. In that case we can apply the same consideration as before, but with adjusted momentum p given by $p^2=2m[E-V(x)]$. The result is the simplest numerical version of the Schrödinger equation in general case

$$\psi(x+\Delta x)=2\psi(x)-\psi(x-\Delta x)-\frac{2m\Delta x^2}{\hbar^2}[E-V(x)]\psi(x) \qquad (5)$$

mentioned earlier – Eq. (2) at the beginning of the paper. But now it was obtained without using derivatives, limits or differential equations. Students used only high school elementary vector algebra and the Pythagorean Theorem.

Equation (5) is mathematically much simpler than differential version of SchE (1). If we know potential energy function $V(x)$, values $\hbar$ and m and we specify the values of E and Δx, then given any two neighboring values of wavefunction $\psi(x)$, mathematically complex numbers and geometrically ordinary arrows, we can find by elementary operations all remaining values - the whole list of all discrete points along the x axis. This means that this process of constructing wavefunctions is simple (no differential calculus or complex numbers) and universally applicable providing an excellent foundation for computer modeling. Moreover nowadays personal computers are sufficient for pedagogical purposes so there is no need for fancy algorithms. To be more precise we need to take only very small step Δx.

III. COMPUTER MODELING: FINDING EIGENFUNCTIONS AND ENERGY LEVELS BY A SPREADSHEET

After the heuristic derivation of the Schrödinger equation (2) students start with computer modeling through a spreadsheet to get intuition and direct experience for stationary wavefunctions – states in a a wide range of one-dimensional potential energy functions. We use Microsoft Excel or Open Office Calc spreadsheets.

Here is a short description of our Excel file Schroedinger.xls and its sheets used by our students. The first sheet of the file includes basic constants and parameters used in modeling. In the second sheet students can interactively change and study corresponding potential energy diagram. The first studied bound system is a potential well with finitely tall walls. The height of the walls can be manually changed to get a variety of situations.

The third sheet is a modeling sheet, where besides table of spatial parameters of a system, potential energy diagram students can see the wavefunction diagram (fig. 4). How do students use this sheet?

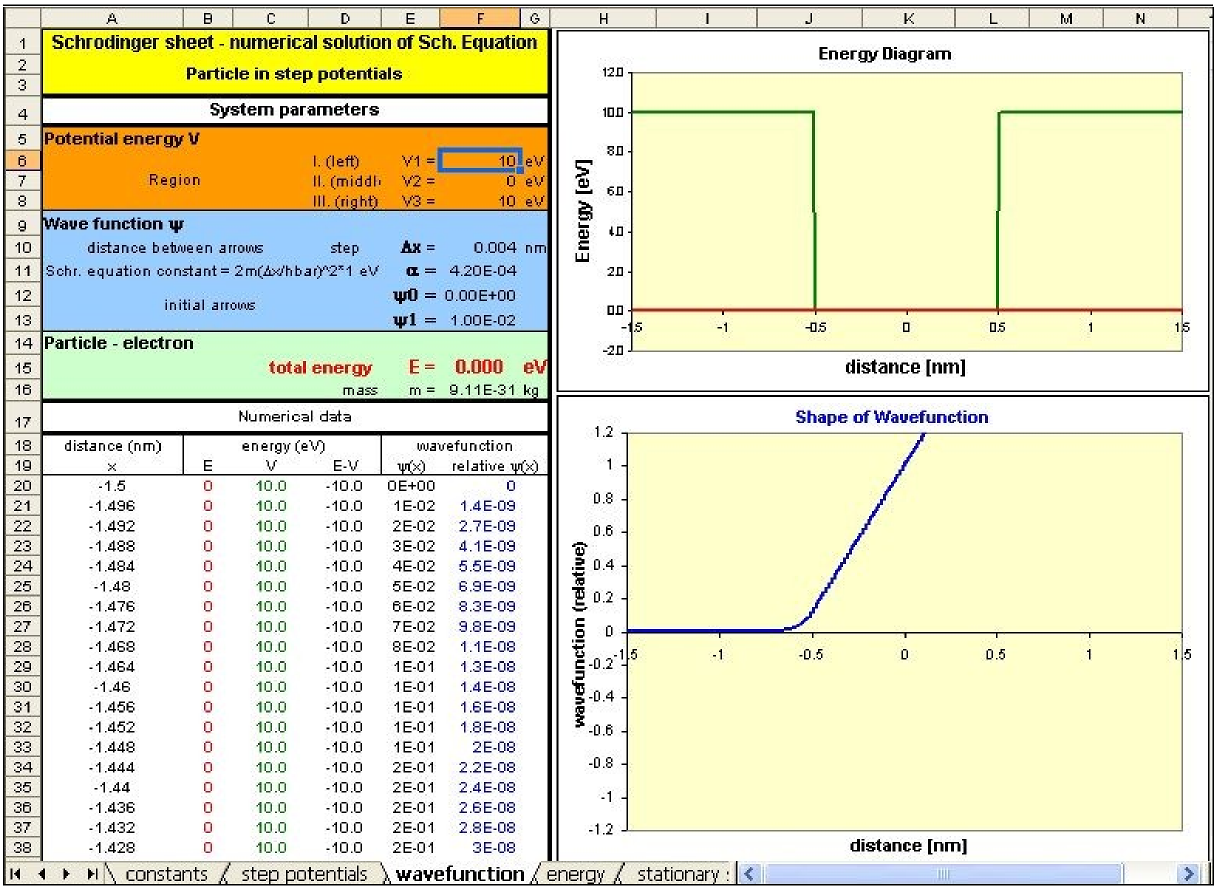

Fig. 4: A screen shot of Schroedinger.xls

Since in computer modeling we were inspired by excellent Thomas Moore's course *Six Ideas that shaped physics* [5], the use is very similar to Thomas Moore's ideas explained in detail in [5], so I shall outline only the main idea. If a student starts with zero energy level (sheet cell the total energy *E*), then according to the wavefunction diagram the resulting wavefunction generated by SchE (5) goes to infinity. (Students have to have in their minds that the diagram in reality includes arrows and for simplicity we do not display the whole arrows, but only their tips creating the blue curve in fig. 5.)

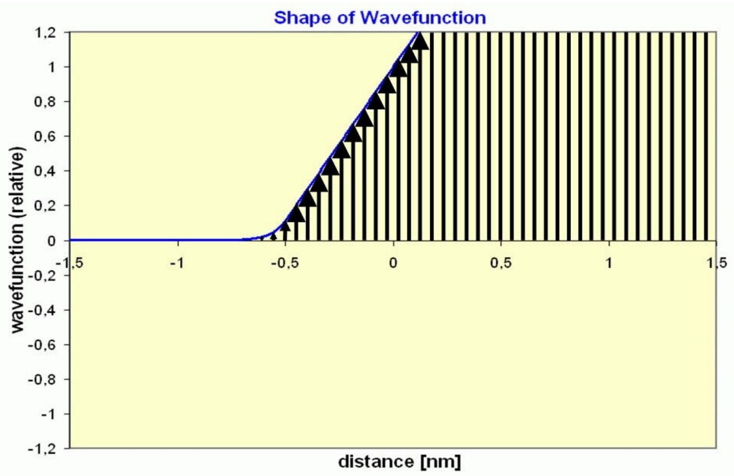

Fig. 5

It is an unrealistic situation from two important reasons. In the right part of space in the wavefunction diagram such wavefunction would imply infinite probability of finding particle in the classical forbidden region, which is clearly absurd. The second important reason is symmetry of the situation, which intuitively requires a symmetric wavefunction. It means the wavefunction should be zero faraway on the right side. If student increases the total energy, he sees that, if the energy is still small the wavefunction "overshoots" zero value as $x \to +\infty$. If energy is too big, the wavefunction goes to minus infinity on the right side. In other words it "undershoots" the condition that it must go to zero as $x \to +\infty$.

By playing, technically called the shooting method standardly used in textbooks based on modeling, e.g. [1] or [5], students found such value of energy level to get the right stationary wavefunction. Using the spreadsheet students can find out all bound states with corresponding energy levels. Fig. 6 shows first four states obtained by this shooting method in Excel .

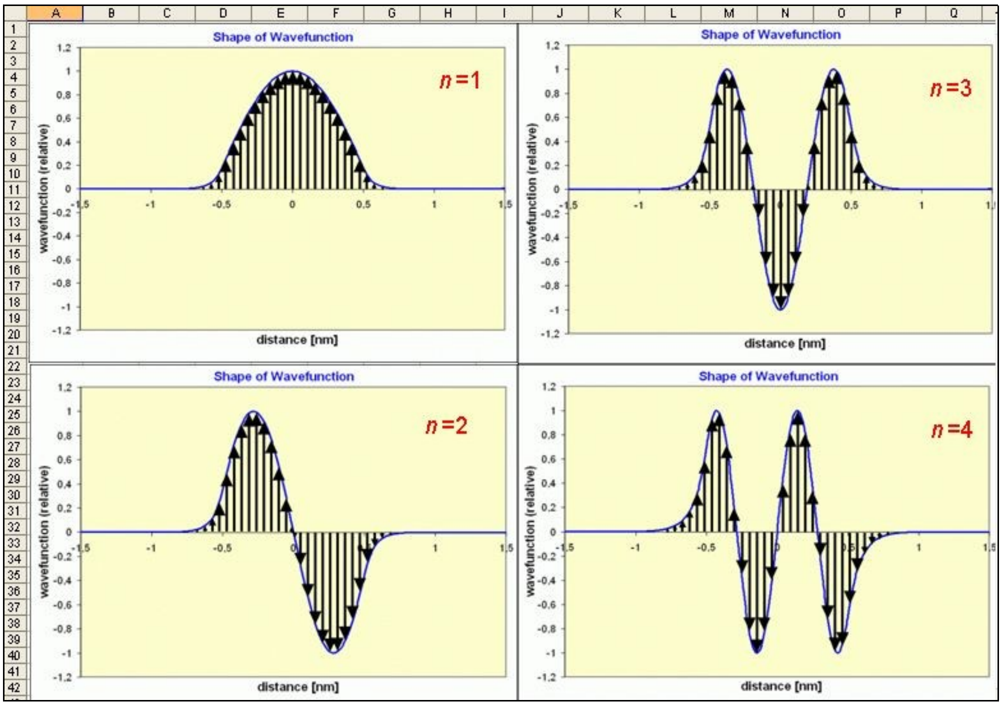

Fig. 6

During this process students also obtain appreciation why energy is quantized and why in a quantum mechanical bound system like potential well a particle cannot have zero energy, which means that the ground state energy is always positive. As precise calculations show it is easy to reach an accuracy better than 1%.

When students understand the crucial idea of a quantum mechanical mechanism for modeling stationary states, later it is more effective and less tedious for students to use a prepared computer program applying the same algorithm as the spreadsheet file. In our case to this moment we use Thomas Moore's piece of software (fig. 7) called SchroSolver [5], which allows to explore many situations in other different one-dimensional potentials. These physically not simplified, but mathematically simple means allow to cover practically majority of themes of introductory quantum courses dealing with stationarity states.

Finally all these tutorials lead students to develop essential prerequisites - skills to learn doing qualitative plots – sketching wavefunctions as it is done with applications of the quantum technology in Witttman at el. *Activity based Modern Physics tutorials* [9].

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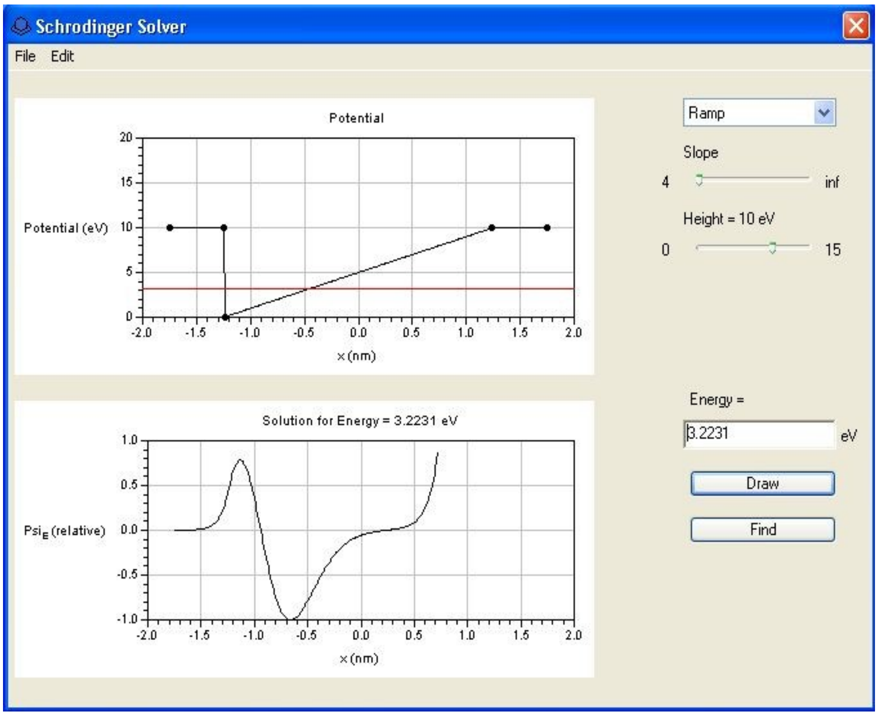

Fig. 7: *A screen shot of Thomas Moore's SchroSolver program for modeling stationary states*

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