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Geometric, noncalculus approach to Schrödinger equation

In contribution we introduce how to conceptually teach and understand the Schrödinger equation from viewpoint of teachers and students without elementary calculus, without complicated postulates, without wave formalism. Our high school and university students, not specialized as majors in physics, are able to derive heuristically the Schrödinger equation only on the basis of high school mathematics, particularly using only vector addition and Pythagorean theorem. Then they study, explore, predict, describe behavior of many important systems of which description can be reduced to one degree freedom description by PC in Excel and Easy Java simulation environment – one of the most modern free tools in modeling for teaching phenomena describable in principle by differential equations.

keywords: Schrödinger equation, conceptual understanding, heuristic geometrical derivation, high school mathematics, PC modeling, Easy Java simulations

Introduction

The fundamental equation of quantum mechanics – the Schrödinger equation, describing and explaining properties of atoms, molecules, and particles of microworld, belongs to very important tools for physicists working in such fields like atomic, molecular, solid state, nuclear and elementary particle physics. The equation is frequently used by chemists in theoretical chemistry, both organic and inorganic, and it appears also in works of molecular biologists.

In terms of analogy we can say that the meaning of the Schrödinger equation in quantum mechanics is equally fundamental as the meaning of Newton's second

law in classical mechanics. However the mathematical difficultness and abstractness of the Schrödinger equation goes significantly behind difficultness of Newton's second law and this situation is evident even in the simplest applications of both laws.

In the paper we briefly present main ideas of our approach to the Schrödinger equation which was tested by us last three years at P.J. Safarik University (the first remark about our work is in [1]). As our experience proves, our approach is appropriate for lower undergraduates at universities, but it is suitable also for last year of high schools in special, not obligatory subjects called physics seminars.

From mathematical viewpoint our approach decreases significantly difficulty of used mathematical ideas, so there are no differential or integral calculus, no differential equations, no complex functions or infinite functional series, no wave formalism, no mathematically difficult postulates.

Instead of that we use only high school vector algebra, geometrical language (elementary trigonometry, properties of sine and cosine functions, Pythagorean theorem) and important part of our approach is simple computer modeling.

Finally our experience shows us that the approach led to higher level of conceptual understanding than it is typical in traditional approaches and it is beneficial for future high school physics teachers and we believe that it can be beneficial also for future chemists, biologists and engineers or in other words for students without strong mathematical background.

Main ideas

How did we achieve such approach characteristics mentioned above? Here is a list of important ideas implied in our approach:

- Firstly we use complex numbers only implicitly in the form of vectors, whose geometrical view was established by Friedrich Gauss many years ago. We call vectors used in quantum mechanics *quantum arrows*.

The only thing needed to know from complex numbers mathematics are two basic operations with quantum arrows: *sum* of quantum arrows identical with the standard vector addition and *product* of quantum arrows, where result is a final arrow whose length is equal to product of lengths of multiplied arrows and angle is sum of angles (Fig. 1).

For effective record of discovered results students are introduced by four special unit arrows with angles 0°, 90°, 180°, 270°: 1, *i*, -1, -*i*. From the arrow product definition and hands-on computer activities students themselves easily formulate a conclusion that multiplication by these arrows only rotates multiplied arrows, so it is a very natural to call them *rotators*. Students also understand properties and reasons for symbols of these rotators.

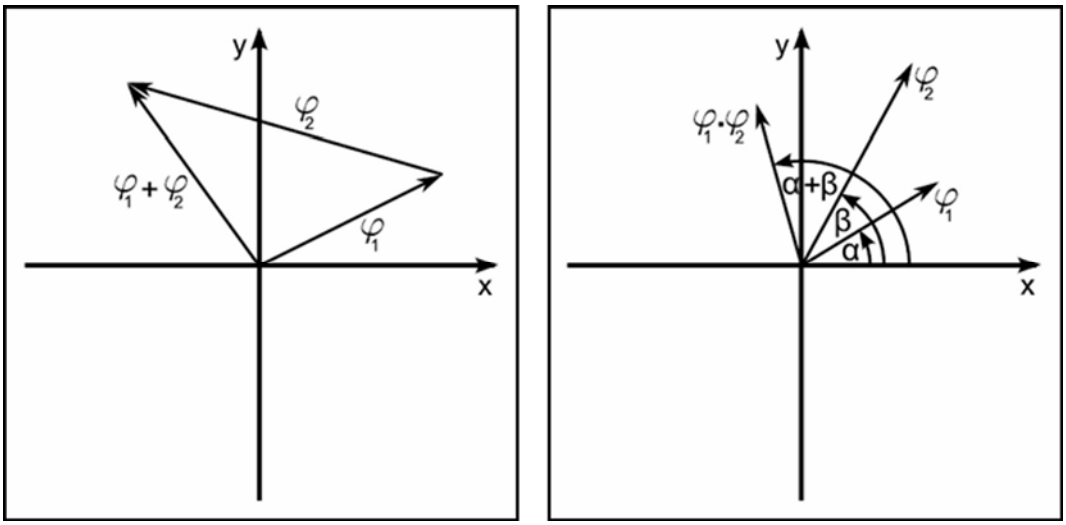

Fig. 1 Graphical display of quantum arrow sum and product .

- The second important idea of our approach is using not Schrödinger or Heisenberg, but Feynman's amplitude version of quantum mechanics. More about basic ideas of this approach in teaching quantum mechanics can be found in references [2-5] or in our review of them in [6]. The idea not to avoid complex numbers and to use only their geometrical form just comes from references [2-5].
- The third idea were very instructive and beautiful Linus Pauling's explanations [7] in quantum mechanics dealing with basic quantum concepts or energy quantization.
- The last important idea is using simple computer modeling, which is now very important part of physics teaching. We decided to use Easy Java simulations [8] – modern and very successful environment for very rapid development of Java applets for science. However all our results can be easily implemented in Excel.

Illustration of our approach – heuristic derivation of Schrödinger equation

In this section we present a brief summary how students make a model for stationary states or find the time-independent Schrödinger equation. (The detailed account of the approach will be submitted for publication in the European Journal of Physics [9]).

Starting point for motivating and heuristic derivation of Schrödinger equation is the same as in traditional courses – the de Broglie hypothesis, which in typical traditional course is e.g. formulated as: „ in 1923 French physicist L. de Broglie proposed that to a beam of any kind of free particle that carries momentum *p* and

energy E there is associated a planar wave with frequency $f = E/h$ and wavelength $\lambda = h/p$." Symbolically:

$$\psi(x,t) = Ae^{(i/\hbar)(px-Et)} \tag{1}$$

However in our approach the de Broglie hypothesis is a consequence of basic postulates of the Feynman quantum mechanics and students are able to discover the following operational description of quantum behavior of free electrons, which increases importantly conceptual understanding what the de Broglie wave is (this scheme is applied also in the new edition of [3]):

1. An electron of momentum p is emitted by a monochromatic source and is detected at a certain place and time.
2. Imagine the electron taking every possible path from the source to arrive at that place and time. The longer the path, the earlier the time at which the electron will have to be emitted. How much earlier depends on the speed of the electron.
3. For each path, there is a combined quantum arrow that describes the whole process of emission, travel and detection. The quantum arrow can be thought of as making one turn for each distance h/p along the path.
4. Add up the quantum arrows for all possible paths, tip to tail, to get their resultant arrow.
5. From the square of the resultant arrow, calculate the probability of detection of an electron.

Now if we consider detections of electron from a monochromatic source in one dimensional case in whole space, then applying first four steps from the previous list, students easily get a picture of the de Broglie wave (Fig. 2).

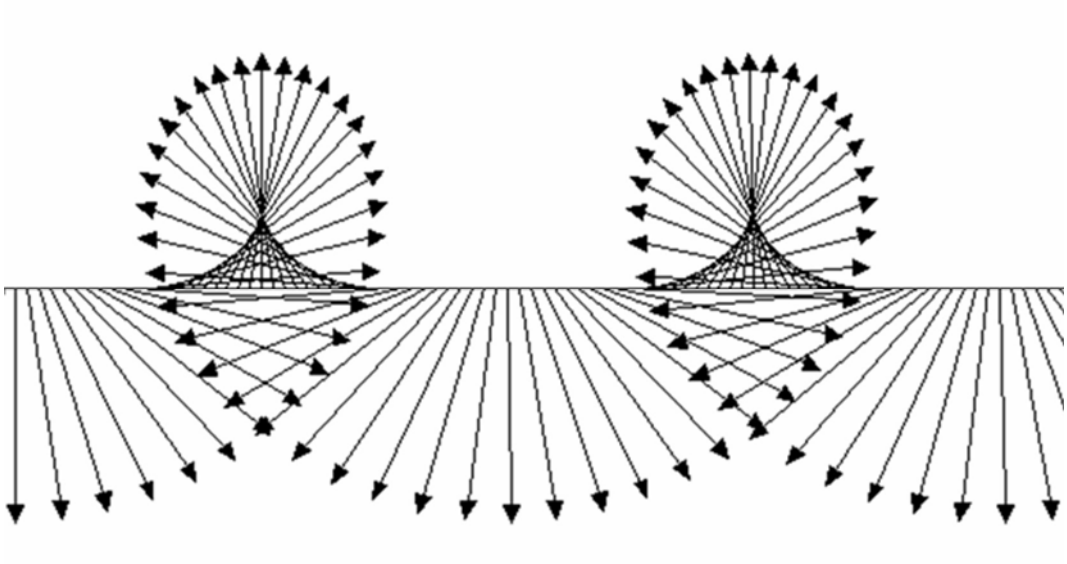

Fig. 2. Pattern of the de Broglie wave (1) at certain time. As time goes on the whole pattern propagates toward positive *x*. From this picture students naturally see why this set of arrows is called the de Broglie weave, because it really behaves like wave. The de Broglie wave is not a graph of sine or cosine as it is depicted in traditional courses. These functions are only real or imaginary parts of the wave.

After constructing de Broglie wave on basis the Feynman version of quantum mechanics, students with the help of tutorials and elementary trigonometry derive a relation between any three close arrows in the wave, which gives them a local description of the de Broglie wave (details see in [1]) or stated another way – an increment version of the Schrödinger equation for free particles or after generalizing to the Schrödinger equation for general case with varying potential energy $V(x)$:

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

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

This version of the Schrödinger equation gives students tool for finding stationary states described by the following algorithm (so-called shooting method), which is implemented by students in Easy Java Simulations environment (Fig. 3) or Excel ([1]):

1. Choose energy E for a required state $\psi(x)$.
2. Generate a list of $\psi(x)$ – first two ones are $\psi(x_0) = 0, \psi(x_1) = 1$

$$\psi(x_{j+1}) = 2\psi(x_j) - \psi(x_{j-1}) - \frac{2m\Delta x^2}{\hbar^2}[E - V(x_j)]\psi(x_j)$$

3. Check auxiliary conditions of physical reasonableness.
4. Repeat algorithm if the conditions are not satisfied.

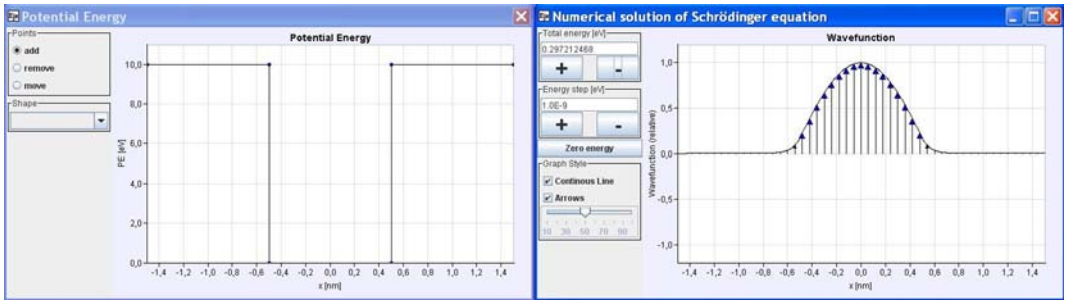

Fig. 3 Finding stationary states in Easy Java simulations environment according to mentioned algorithm using an increment version of the Schrödinger equation.

Then students use this algorithm to explore and to understand conceptually and quantitatively several important applications like quantum well lasers, hydrogen atom, chemical bond, quantum band conductivity.

Finally using tutorials students derive in similar geometrical way and also use an algorithm, at same level of difficulty as previous one, for time development of any initial wave function:

1. Choose (reasonable) initial state ≡ list of $\psi_{t-\Delta t}(x_j)$.
2. Calculate state $\psi_t(x_j) = \psi_{t-\Delta t}(x_j) - i\left(\frac{\Delta t}{\hbar}\right)H\psi_{t-\Delta t}(x_j)$.
3. Update state every Δt as

$$\psi_{t+\Delta t}(x_j) = \psi_{t-\Delta t}(x_j) - i\left(\frac{2\Delta t}{\hbar}\right)H\psi_t(x_j),$$

where $H\psi_t(x_j) \equiv \frac{\hbar^2}{2m\Delta x^2}[\psi_t(x_{j+1}) - 2\psi(x_j) + \psi(x_{j-1})] + V(x_j)\psi_t(x_j)$.

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