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Time-dependent scattering in 3D

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Quantum mechanics is a difficult part of undergraduate physics courses both conceptually and mathematically. Numerical solution of problems on a computer drastically widens the assortment of the few problems that can be solved analytically, and it opens the possibility of the study of more realistic systems as well. The presentation of the results in a graphical form contributes to the understanding of the concepts and phenomena studied. Animation is a unique tool in the study of time dependent phenomena: the images calculated at different time instants may be joined as a movie. In the middle of nineties the performance of personal computers and workstations combined with efficient numerical techniques opened new perspectives for teaching quantum mechanics, in particular time-dependent scattering. Their recent performance allows to extend the calculation from 2D to 3D and investigate phenomena like the transmission of electrons through carbon nanotubes.

INTRODUCTION

Students of electrical engineering at the Budapest University of Technology and Economics (former Technical University of Budapest) study Physics in three semesters. While classical physics is taught in the first two semesters, the third semester is devoted to modern physics. About two third of the third semester consists of a quantum mechanics course based on traditional axiomatic treatment.

Quantum mechanics plays a fundamental role in the description and understanding of most natural phenomena. The properties of atoms and phenomena which occur on atomic scale, as the propagation of electrons in a crystal, the operating principle of solid state electronic devices, etc., cannot be understood and explained in the framework of classical physics. On the other hand, nowadays the basic knowledge of the concepts of quantum mechanics and its laws is an integral parts of the human culture and is a must for everyone who intends to have an idea and a certain understanding about how Nature works. Therefore we strongly believe that quantum mechanics and an introduction into solid state physics are essential parts of the physics curriculum for students of the Electrical Engineering Faculty.

WHY IS QUANTUM MECHANICS DIFFICULT FOR STUDENTS?

On the other hand, quantum mechanics is one of the most difficult parts of undergraduate physics courses both conceptually and mathematically [1]. This may cause serious difficulties for an average student in acquiring the subject. We are facing this problem especially since the number of students has largely increased, along with the lowering of the entrance requirements in math and physics.

Most students find quantum mechanics too abstract and mathematically difficult. There are several reasons for this and some of them are quite obvious. First the learning process of the concepts and laws of classical physics, in particular classical mechanics, is strongly supported by the everyday experience of the student which can be enhanced by classroom demonstrations and by performing direct and simple experiments. Understanding of the concepts and principles can be further deepened

by problem solving. It is supported by the wide assortment of examples and problems available in the textbooks.

In classical mechanics the description of the dynamic state of a particle at a given time t is based on the specification of six parameters: the components of the position $\mathbf{r}(t)$ and linear momentum $\mathbf{p}(t)$ of the particle. All the dynamical variables (energy, angular momentum, etc.) are determined by the specification of $\mathbf{r}(t)$ and $\mathbf{p}(t)$. Newton's laws enable us to calculate $\mathbf{r}(t)$ through the solution of a second order differential equation with respect to time. Consequently, they fix the values of $\mathbf{r}(t)$ and $\mathbf{p}(t)$ for any time t when they are known for the initial time.

All this is essentially different for quantum mechanics. The main difficulty is caused by the fact that we do not have direct sensory experience about particles and systems on the atomic and subatomic scale. The particles do not obey the laws of classical mechanics; the extrapolation of the behaviour of macroscopic objects to the microworld is erroneous. The classical mechanical description breaks down; basic concepts, as mass point localised in space, trajectory of a particle, etc., cannot be used. The quantum mechanical description of physical systems differs radically from the one provided by classical mechanics (although the latter constitutes, in numerous cases, an excellent approximation).

A more complicated description of phenomena must be used in quantum mechanics. The dynamic state of a particle, at a given time, is characterised by a *wave function* $\Psi(\mathbf{r},t)$, which contains all the information that is possible to obtain about the particle. The state no longer depends on six parameters, but on an infinite number of parameters: the values of the complex valued wave function $\Psi(\mathbf{r},t)$ at all points $\mathbf{r}$ in the coordinate space. For the classical idea of trajectory (the succession in time of the various states of the classical particle) we must substitute the idea of the propagation of the wave associated with the particle. $\Psi(\mathbf{r},t)$ is interpreted as the *probability amplitude of the particles presence* and $|\Psi(\mathbf{r},t)|^2$ is the probability density of the particle being, at time t, in a volume element dr^3 situated at the point $\mathbf{r}$.

The equation describing the evolution of the wave function $\Psi(\mathbf{r},t)$ is the time-dependent Schrödinger equation. The Schrödinger equation is a second order linear differential equation; the linear superposition of its solutions leads to interference effects. It is of first order in t; from this it follows that, given the initial state $\Psi(\mathbf{r},t_0)$, the final state $\Psi(\mathbf{r},t)$ at any subsequent time t is determined. There is *no indeterminacy* in the time evolution of a quantum system.

Indeterminacy appears only when a physical quantity is *measured*, the wave function then undergoes an unpredictable modification. However, between two measurements, the wave function evolves in a perfectly deterministic way, governed by the Schrödinger equation. The result of a measurement of an arbitrary dynamic variable must belong to the set of the eigen values of the operator representing the dynamic variable. With each eigen value it is associated an eigenstate, the eigen function of the operator belonging to the particular eigen value. If a measurement yields a particular eigen value, the corresponding eigen function is the wave function of the particle immediately after the measurement. The predictions of the measurement results are only probabilistic: they yield the probability of obtaining a given result in the measurement of a dynamical variable.

For an average engineering student the understanding of the complicated concepts, terminology and language of quantum mechanics is a hard job. The learning process is not supported by the everyday experience and there are only few experiments available for classroom demonstration, but even for these (as for instance electron diffraction) the interpretation of the results is not trivial. As the state function (the complex probability amplitude) cannot be measured directly, its properties have to be inferred from experiments involving the measurement of counting rates in scattering experiments, measurement of optical spectra, etc.

A further difficulty arises from the fact that only a limited number of problems are available for the students to practice. The number of cases when an analytical solution does exist is very limited; the solution of nontrivial problems takes a long time and requires appropriate mathematical skills, beyond that, these skills cannot be expected from an average engineering student. In spite of that, it is important for the students to get acquainted with many different cases and their solutions, in order to get the hang of quantum phenomena.

COMPUTER SIMULATION AS AN EFFICIENT LEARNING AID

Numerical solution of problems on a computer drastically widens the assortment of the few problems that can be solved analytically, and it opens the possibility for the study of more realistic systems as well. By performing "computer experiments" or at least by studying the outcomes of computer simulations students can get a certain experience in quantum mechanics. The presentation of the results in graphical form may contribute to a large extent to the understanding of the concepts and phenomena studied.

Time-dependent Scattering

For many students it is difficult to imagine how a wave packet evolves in time, how it propagates and spreads out, what goes on, when it approaches a potential barrier, what happens to it during the interaction and how the reflected and transmitted wave packets are formed, etc. In order to follow how the state of a system evolves in time, one has to solve the quantum mechanical equation of motion, the time-dependent Schrödinger equation. However, there are only few and oversimplified cases for which this can be done analytically. Therefore, numerical simulation is a unique tool in the study of time dependent phenomena. Further more the images calculated at different time instants may also be used for animation, as it has been done in Ref. [2] where the graphical output of a main frame computer was used to produce a movie for scattering in one dimension. The series of snapshots showing the scattering process of a 1D Gaussian wave packet on a potential barrier can already be found in the recent textbooks of quantum mechanics.

Nevertheless, for more or less realistic systems the numerical solution was also a difficult task because of hardware and software limitations. In the nineties these limitations were largely removed by the efficient numerical techniques developed and by the high speed and performance of workstations and personal computers. These computational advances made it possible to introduce the time dependent quantum mechanical study of two dimensional (2D) systems into the education as well [3,4]. An efficient numerical technique, the split operator Fourier transform method has been used for the solution of the 2D time dependent Schrödinger equation in which the time evolution operator is approximated by the symmetrical unitary product

$$e^{-i\mathbf{H}d_t/\hbar} \approx e^{-i\mathbf{T}d_t/2\hbar} e^{-i\mathbf{V}d_t/\hbar} e^{-i\mathbf{T}d_t/2\hbar} \quad (1),$$

where **H** = **T** + **V** is the Hamiltonian operator of the system, **T** and **V** are the kinetic and potential energy operators, respectively, and δ_t is the time increment. According to (1), the evaluation of the action of the evolution operator on the wave function is split into three consecutive steps. The potential energy operator of the system is a scalar function in coordinate space thus the effect of the propagator on the wave function is a simple multiplication by $e^{-iVd_t/\hbar}$. In the evaluation of the effect of the propagator $e^{-i\mathbf{T}d_t/2\hbar}$ on the wave function the property of Fourier transform is utilised that differentiation of a function in coordinate space is equivalent to multiplication of the function's representation in the Fourier transform space (**k** space) with the conjugate variable *k*. In the **k** space the kinetic energy operator is a scalar function of the wave vector ($T = \hbar^2 k^2 / 2m$), thus the action of the exponential containing the kinetic energy operator on the wave function can be evaluated as

$$e^{-i\mathbf{T}d_t/2\hbar}\Psi(\mathbf{r},t) = \mathrm{F}^{-1}\left[e^{-i\hbar k^2 d_t/4m}\mathrm{F}\left[\Psi(\mathbf{r},t)\right]\right] (2),$$

where the Fourier transform is denoted by F and the inverse Fourier transform by F^{-1}. The evolution of the wave function over a time increment δ_t is calculated in a straightforward way: first equation (2) is applied, then the result is multiplied by $e^{-iVd_t/\hbar}$ and finally equation (2) is applied again. Thus the evolution is approximated by the product of a free particle evolution for one-half the time increment, a potential only evolution for a full time increment, and a final free particle evolution for another half time increment. Fast Fourier transform (FFT) is used to perform the Fourier integrals. Attention must be paid to the fact that FFT views both coordinate (**r**) and **k** space (Fourier transform space) discretely and presumes the periodicity in the function. The detailed description of the physical and mathematical background is given in Ref. [4].

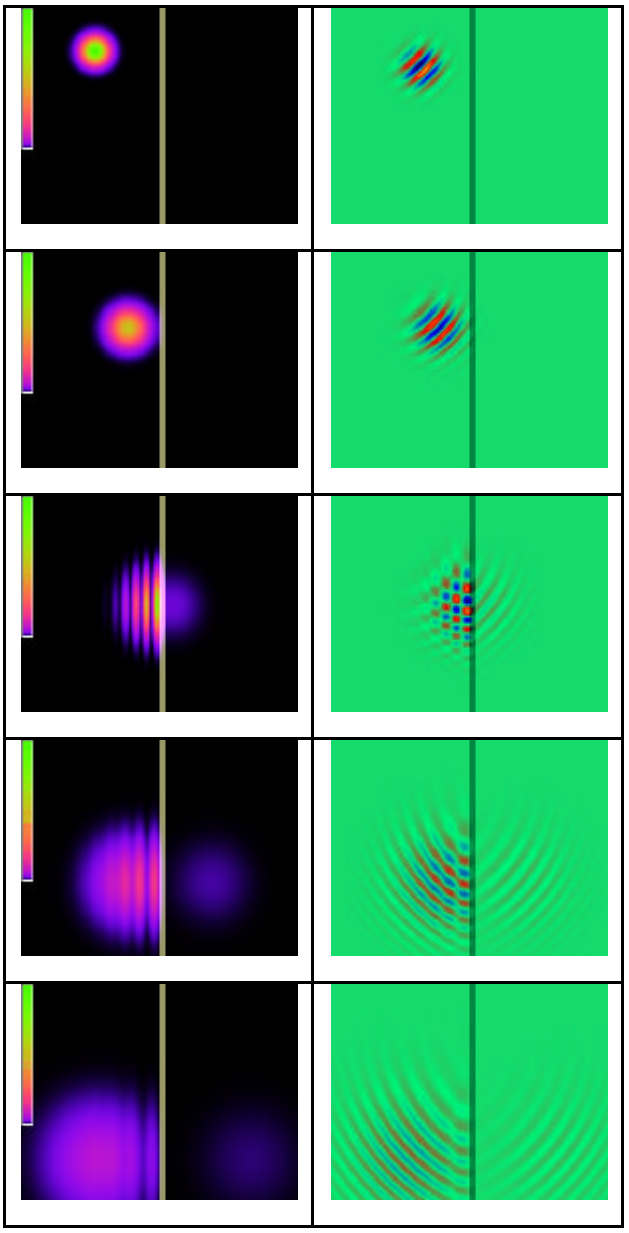

FIGURE 1. Time evolution of the 2D Gaussian wave packet tunneling through a potential barrier. The barrier located in the middle of the figures is denoted by a grey vertical stripe. The probability density is shown on the left row at different time instants, the real part of the wave function on the right row. The real part shows the wave nature of the wave function, the distance between the wave fronts is the wavelength. Interference patterns are seen in the probability density while the wave packet is interacting with the barrier.

Time-dependent Scattering in 2D

For the calculations of the evolution in time of two dimensional Gaussian wave packets a 512 $\times$ 512 grid was used to span the region of coordinate space of 256 $\times$ 256 atomic units (Bohr radius = 5.291772 $\times$ 10^{-11} m). The number of points in the **k** space was also 512 $\times$ 512. The time increment δt was chosen to 0.3 atomic time unit (7.2 $\times$ 10^{-18} s). The probability density function $|\Psi(\mathbf{r},t)|^2$ and the real part of the wave function $\mathrm{Re}(\Psi(\mathbf{r},t))$ are shown in the form of 2D color graphs (displayed at different time instants) which can also be used for computer animation.

Calculations of time-dependent scattering on different potentials were performed. One of the results, the evolution of a Gaussian wave packet tunnelling through a potential barrier is demonstrated in Figure 1. The particle is approaching a thin rectangular potential barrier (of 3 Bohr) separating the two regions. Classically, the kinetic energy of the particle is not enough to pass the potential barrier (it is less than the height of the barrier). When the wave packet is moving toward the potential barrier in the constant (zero) potential region its shape does not change, except it is spreading out. When the leading edge of the wave packet reaches the potential barrier oscillations occur in the wave packet caused by the interference between the incident and reflected waves. After a transitory period the wave packet splits into two. The reflected wave packet is returning to the left. The second one, the transmitted wave packet of probability propagates towards the right, demonstrating that there is a finite chance for the particle to tunnel through the classically forbidden region. Computer animation showing the details of the tunneling process (and scattering on other potentials) is available on the web [5].

Time-dependent Scattering in 3D

Recently the investigation of nanostructured materials is a subject to great interest. Scanning tunneling microsocpy (STM) provides information both about the topographic and electronic structure on the nm scale. However, because of the complex geometry of the system, the interpretation of the images is delicate. Due to this, computer simulation of the tunneling process is an important tool in understanding the

measured results. This can be done by the numerical solution of the time-dependent Schrödinger equation. In many cases, depending on the geometry and symmetry of the arrangement, results of the 2D calculations provide valuable information. But in lack of symmetry only the solutions in three dimensions provide a full picture of the tunneling process. Although it requires much more computation, the job can be done on the recent powerful personal computers. A nice example is the 3D time dependent study of the tunneling of the electron wave packet through a supported carbon nanotube in the STM [6].

Study of electron transport through carbon nanotubes is of great scientific and practical importance because their interesting electronic properties make them one of the building elements of future nanoelectronic devices.

The model system geometry used in the calculation is shown in the upper left panel of Figure 2. The carbon nanotube is modeled by a cylinder of 0.5 nm radius floating above the support plane at a distance of 0.335 nm. The STM tip is taken as a hyperboloid of 0.5 nm apex radius. The chosen value of 0.4 nm for the tip - carbon nanotube tunnel gap is consistent with that estimated from the STM experiments. A two-valued potential was used as a model of the STM tip - nanotube - support system. The potential is zero in the vacuum and –9.81 eV inside the tip, below the support surface and between a 0.142 nm thin cylindrical layer centered on the tube. See Ref [6] for details.

By numerically solving the time-dependent 3D Schrödinger equation the evolution of a Gaussian wave packet approaching the tunnel junction from inside of the tip bulk was calculated. The time dependent probability density function, $|\Psi(\mathbf{r},t)|^2$ is visualised by snapshots of a constant density surface in Figure 2. In the panel t = 0.0 fs of Figure 2 the initial wave packet is shown. The sphere surface is clipped at the upper boundary of the presentation box. At t = 1.4 fs the wave packet has already penetrated into the tip apex region. The part reflected back into the tip bulk forms interference patterns with the incoming wave. A fraction of the wave packet just begins to enter into the tip - carbon nanotube interface. At t = 2.1 fs the wave packet flows around the tube and simultaneously tunnels through it. The incoming and outgoing waves form interference patterns in the tip apex region.

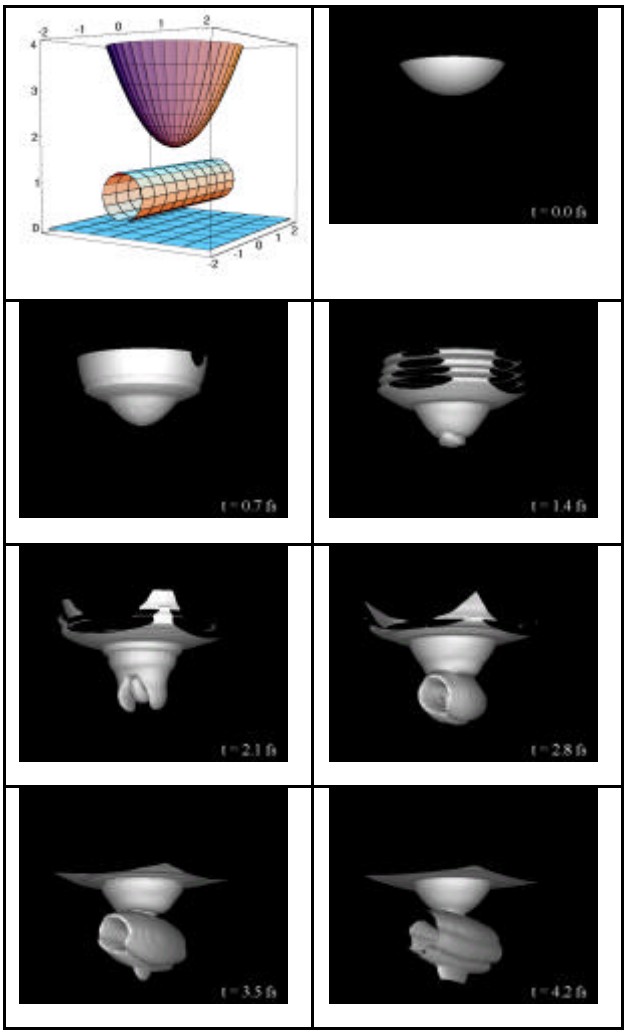

FIGURE 2. Time evolution of the probability density of the 3D wave packet approaching the STM junction from the tip bulk and tunneling through the nanotube into the support. The upper left image is the model system used in the calculation. The labeled box is the presentation box. All dimensions are in nm. The subsequent images show snapshots of a constant probability density surface. This surface is clipped at the presentation box boundaries (upper, lower, right, left, front, rear).

When the two wave packet parts (one moving on the left side and another on the right side of the tube) meet at the lowest point, standing wave patterns begin to form along the tube circumference. Subsequently the wave packet tunnels through the carbon nanotube - support

junction and enters into the support surface (at t = 3.5 fs). In the meantime the probability density is gradually spreading along the tube axis. At t = 4.2 fs the carbon nanotube - support tunnel channel begins to open along the tube axis. The 3D tunneling calculation made it possible for the first time to study the phenomenon of wave packet spreading along the carbon nanotube during the tunneling event. This spreading can explain the features of the STM image. Computer animation showing the details of the tunneling process is available on the web [7].

CONCLUSIONS

High performance personal computers and workstations combined with efficient numerical techniques opened new perspectives for teaching quantum mechanics, in particular time-dependent scattering. The presentation of the results obtained in a graphical form contributes to the understanding of the concepts and phenomena studied; the images calculated at different time instants can be used for animation. Recently the solution of the 3D time-dependent Schrödinger equation is already a reality as it has been demonstrated on the example of the simulation of tunneling of electrons through carbon nanotubes in a scanning tunneling microscope.

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