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Educational reconstructions of quantum physics using the sum over paths approach with energy dependent propagators

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Abstract. Moving from the research tradition on the use of Feynman's sum over paths approach in education, we have developed an educational reconstruction of elementary quantum physics which uses Feynman paths at fixed energy and is capable of a simple conceptual explanation of discrete energy levels in bound systems. The reconstruction has been found to offer several educational advantages, may help students think of quantum physics in a way more akin to how the subject is used by scientists, and allows to shed light on the relationship between energy and time.

1. Introduction

In the traditional teaching of physics in the secondary school, energy is usually first taught as an ancillary concept in kinematics, where students have to deal with problems concerning the time evolution of pointlike masses, and energy is only marginally useful. Gradually, as students proceed onwards in the physics course, energy takes more and more importance, and they should be led to reflect upon the circumstance that, in all the problems in which time is irrelevant (for example, problems of equilibrium thermodynamics) energy is the central concept to be considered for understanding the behavior of a system.

It would be desirable that in the final year of secondary school, when students are introduced to rudiments of quantum physics, such introduction was done first of all in the energy domain, i.e. starting from stationary problems. This is consistent with the fact that, also in introductory University courses, which however typically use a Schrödinger equation approach, students first encounter stationary problems. Not only are time independent, fixed energy problems easier to solve in quantum physics; they are also those on which the theory gained its first historical successes (for example, the explanation of the photoelectric effect and the derivation of the energy levels of hydrogen-like atoms).

The research line on the use of Feynman's sum over paths approach in education, started from the work of E. F. Taylor [1], has had important successes in the past, especially in leading students to build a qualitative, conceptual understanding of the basic meaning of the theory. However, Taylor's educational reconstruction, following the route tracked by Feynman's 1948 paper on path integrals [2], and the divulgation book QED [3], was formulated in the time domain, starting from the time-dependent single particle propagator. A problem of such approach is that even a conceptual treatment of simple bound system becomes rather intricate.

In the last few years, our group provided an innovative contribution by reconsidering the educational proposals based on sum over paths, re-elaborate and extend them using a fixed energy (time-independent) sum over paths approach [4]. The theory of energy dependent propagators (or Green



functions) in nonrelativistic quantum mechanics started from the works of M. Gutzwiller in the 1970's [5], and has allowed to obtain several results of theoretical interest. Translating such approach to an educational reconstruction essentially allowed us to preserve all the advantages of the traditional sum over paths approach, and also to obtain a conceptually clear treatment of the emergence of discrete energy level in bound systems, and of the time-energy uncertainty relationship.

The discussion of the approach is supported by a collection of interactive simulations, realized in the open source GeoGebra environment, which we used to assist students in learning the basics of the method, and help them explore the proposed experimental situations as modelled in the sum over paths perspective

2. The time-dependent sum over paths approach in Physics education research

The sum-over-paths approach to quantum mechanics has been explored by a number of physics educators, aiming at an elementary introduction to quantum physics using the conceptual tools of Feynman's path integral formulation[7-11].

The conceptual understanding of single-particle quantum physics that is provided by the sum-over-paths approach, in the usual time-dependent version, can be summarized as follows:

- i. The quantum object goes through all possible paths from an initial space-time point (x_i, t_i) to a final space-time point (x_f, t_f) .
- ii. A complex number, often represented by a conventional rotating vector, is associated with each of the paths; its phase angle is proportional to the classical action, $R = \int L(t) dt$, calculated along the path.
- iii. The (normalized) sum of all contributions from the possible paths starting at (x_i, t_i) and ending at (x_f, t_f) gives the time-dependent propagator, which can be understood as the probability amplitude of finding at (x_f, t_f) a quantum object that was initially at (x_i, t_i) .
- iv. The probability P of detecting the quantum object at (x_f, t_f) is then computed by taking the square modulus of the propagator.

In the last twenty years, authors have proposed and experimented with several versions of this approach, [7-11] especially in university education for non-specialists,[12] and in high school.[13] In these settings, in fact, use of less advanced mathematics is normally in order, and the ability to solve problems may be partly sacrificed in favour of a clear understanding of the fundamental structure of quantum theory.

Thus the approach was in general judged advantageous by Physics education researchers even if the usual time dependent formulation of sum over paths can also give rise to some difficulties, many of which are known already from the initial work of Taylor[1].

Among these difficulties we underline:

- A time-dependent formulation may increase students' confusion between the concepts of quantum paths and classical trajectories
- The time-dependent treatment obscures the fact that many of the most important predictions of quantum physics are actually time-independent statistics. For example, the treatment of elementary one-dimensional stationary problems is intricate. Finding the eigenfunctions for confining potentials usually requires computing the time-dependent propagator and then determining the initial amplitudes that, for the given propagator, are stationary in time.

In order to clarify the problem concerning the stationary or time dependent phenomena we can analyze the case of the two slit interference of an individual electron.

This problem can be treated in the sum over paths perspective in two ways:

- a) Considering an initial wavefunction (a "wavepacket") and evolving all the points belonging to it using Feynman's path integral propagator.
- b) Considering the time independent problem (at fixed energy) of the propagation of a quantum object from the source to the detector, and using the time independent propagator (green function) which basically (apart from a prefactor) reduces to e^{ikx}

The latter approach may be called “stationary path integral” and the results of the two methods agree, if the energy time-dependent wavepacket in method a) is defined with sufficiently small uncertainty (see e.g. ref.[14]).

3. The time-independent sum over paths approach

In our own approach we treat quantum objects using a sum-over-paths approach at fixed energy, independent of time. More explicitly, the sum-over-paths approach at fixed energy, for time-independent problems, can be compactly described as follows:

- i. The quantum object goes through all possible paths at fixed energy E from an initial point in space x_i (the source) to a final one x_f (the detector).
- ii. A complex number whose phase angle is proportional to the classical abbreviated action $S = \int p(x) dx$ calculated along the path, where $p(x)$ is the particle momentum at point x .
- iii. The sum of all contributions from the possible paths at fixed energy starting at x_i and ending at x_f gives the energy-dependent propagator, or Green function, which can be understood as the probability amplitude of finding at x_f , a particle with defined energy whose source is at x_i , independently of arrival time
- iv. The probability \wp of detecting the quantum object at x_f is then proportional to the square modulus of the Green function. For bound systems, the probability is nonvanishing only when the energy E corresponds to an allowed energy level.

In this way, the conceptual structure of Feynman's formulation is entirely preserved, with two main modifications:

- the action R is replaced by the abbreviated action S ;
- all paths connecting x_i and x_f , regardless of travel time, are considered.

The “*disappearance of time*” allows us to introduce the idea (of educational value in itself) that when energy is fixed, time must be completely unknown; and also, to provide an interesting connection with the time-energy uncertainty relationship.

Thanks to this new formulation [15-16] we are able to treat many confined systems of interest, as well as the important case of tunneling, with rather elementary mathematical tools. The approach can be used to solve all problems which are generally treated using the time-independent Schroedinger equation.

When we treat both confined and open systems with piecewise-constant potentials, we obtain exact results. For more complex systems approximate results (at the level of Wentzel-Kramers-Brillouin approximation) are found.

Details and technicalities of this approach are beyond the aims of this work. Here we just present some examples while the accurate discussion about the calculations is reported in refs.[4], [17] and [18].

3.1. The Double slit

An interesting case where the approach is capable of providing a more consistent answer to typical student's difficulties concerns the simple two slits. In the single photon¹ picture the basic problem consists in a source placed at point S, emitting a photon which may or may not be collected at a detector at point P.

According to the original proposal of Feynman the problem is discussed in terms of phases, phasors and paths. The phases are computed over all its possible paths from the source to the detector. Then the corresponding phasors must be summed to find the ‘resulting arrow’ depending on the path length.

A probabilistic interpretation has to be given and the square modulus of the resulting arrow at point P must now be interpreted as (proportional to) the probability of detecting the photon at P.

¹ In this paper we do not go in depth in the minor differences between problems concerning single photons or single electrons, which essentially consist in helping students understand the consequences of the different relationship between wavelength and energy. Generally, our educational paths start with photons, and introduce massive particles later.

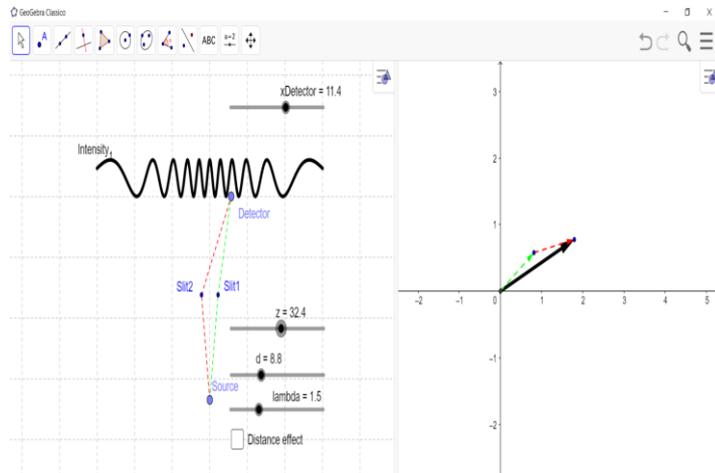


Figure 1 GeoGebra simulation of the two-slit experiment with pointlike slits, illustrating the general structure of most simulations in our collection. In the left window we represent the physical setup (source, detector and other elements of physical reality such as, in this case, the slits and screen). We also display all the possible paths for the quantum object which we include in the computation.

In the right window, the sum of complex amplitudes for all paths at the detector, providing the final amplitude and probability, is represented. The possibility of varying relevant physical parameters and the detector position is provided by sliders and checkboxes.

3.2. Infinite square well

We use the ‘particle in a box’ model as the paradigmatic example for the treatment of bound systems in the sum over paths approach. A quantum object is confined in a square potential well with infinite depth and width L . For a fixed energy E , the particle can reach the detector x_f starting from a source at x_i through one of four families of paths, depicted in Fig. 2.A. The phasor corresponding to each path is computed by the usual rules, with each reflection contributing a π phase loss.

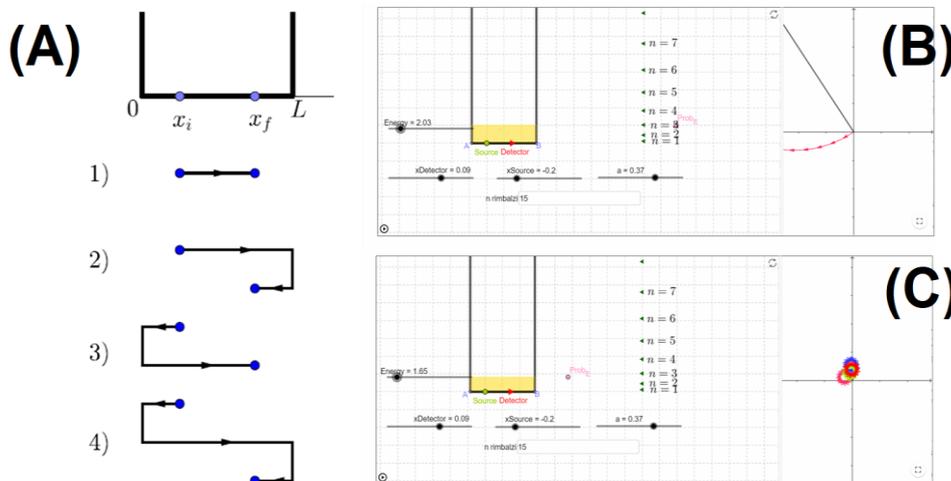


Figure 2 (A) Four basic possible routes exist from the source to the detector: the direct $S \rightarrow D$ path, the $S \rightarrow A \rightarrow D$ and $S \rightarrow B \rightarrow D$ reflected paths, and the $S \rightarrow A \rightarrow B \rightarrow D$ comprising two reflections. Theoretically, all the paths which can be constructed by adding to any of the above an arbitrary number of full back and forth routes should be considered. (Right) Simulation of the infinite square potential well. (B) If the energy corresponds to one of the potential eigenvalues, the paths differing for an integer number of back and forth trips in the hole are in phase, and the corresponding resultant amplitude has a peak (here near the $n=3$ eigenvalue). (C) For all other values, the amplitude in the limit $m \rightarrow \infty$ will vanish.

Allowed energy levels (the poles of the energy dependent Green function [4]) can be determined uniquely from the condition that two paths differing for a full back and forth round trip in the well are

in phase. Thus the full Green function can be determined and the stationary wave functions (eigenfunctions) can be also evaluated.

In order to demonstrate the generality of the method in approaching piecewise constant potentials, we derived the quantization condition for the asymmetric infinite square well or "step in a box" potential. Summing all the paths of the basic families depicted in Figure 3, one can derive the Green function and find the poles.

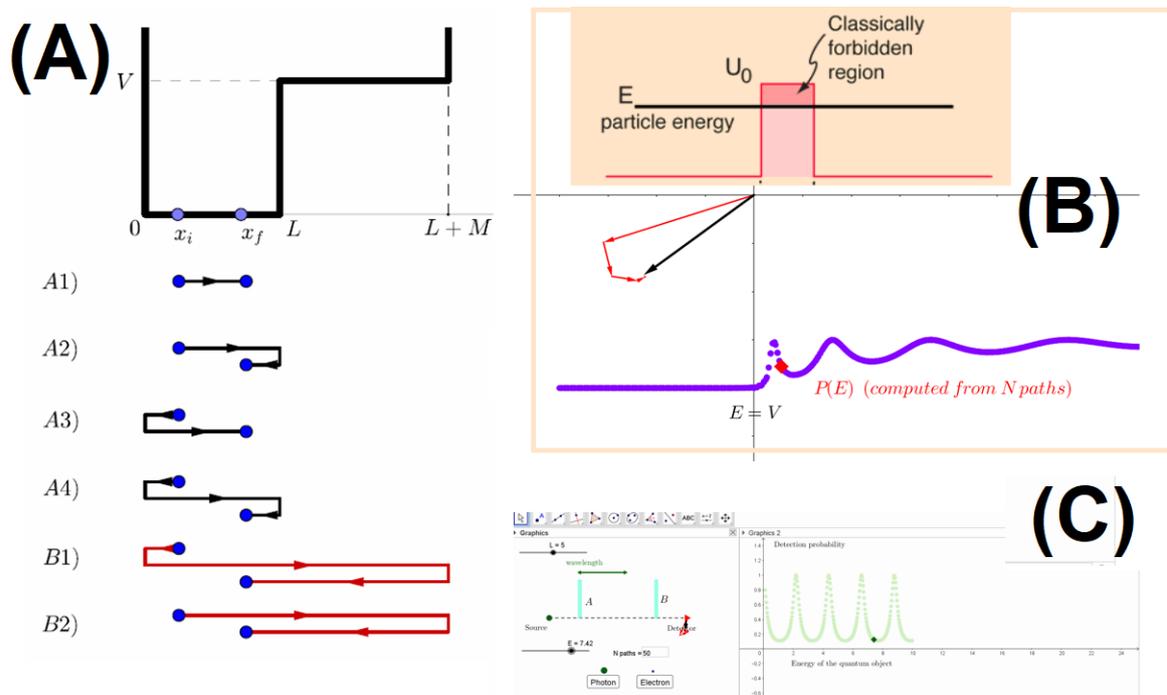


Figure 3 (A) Principal paths for the asymmetric infinite square well potential. Paths A1 to A4 connect x_i to x_f without leaving the left part of the well, while paths B1 and B2 involve a full round trip in the right part of the potential. (B) The transmission probability for a square barrier as a function of energy, computed by using the sum over paths approach in a Geogebra simulation. (C) GeoGebra simulation of an open system displaying resonant tunneling

3.3. Tunneling from a square barrier

The problem of tunneling from a square barrier can also be solved analytically, and the main conceptual elements of the solution (e.g. how to find resonances in transmission probability) can be shown to students through a simulation (Figure 3.B).

3.4. Open resonant quantum systems

A resonant system consisting of a source emitting a photon (or electron) which has to pass through two semi-reflecting barriers to reach a detector. This system can be used as an intermediate step between open and confined systems.(Figure 3.C)

3.5. The time-energy uncertainty relationship

In the fixed-energy sum over paths approach, the uncertainty in the travel time of the quantum object from source to detector is considered infinite. Thus, for bound systems, infinitely many paths, going through an arbitrary number of back and forth roundabouts within the confining potential, need to be considered in order to obtain the allowed energy levels. On the other hand, one may weaken the assumption of infinite uncertainty in travel time, considering only a finite, though large, uncertainty. The logical consequence is to only consider a finite number of paths, namely those whose travel times differ by less than the time uncertainty. The approximate Green function which will result, will not have

sharp divergences, but widened peaks, whose width in energy can be described by a relationship of the kind $\Delta E \cdot \Delta t \approx \hbar$.

This perspective on the time-energy uncertainty relationship is consistent with the accepted interpretation providing, for example, the "natural width" of atom emission peaks

Details of the calculations depend on the system considered, but are very similar. One of the simplest case is the particle on a ring. Here, a finite time uncertainty leads to consider, for each value p of the momentum of the quantum object, a number of possible paths

$$N \approx \frac{p\Delta t}{\pi mR}.$$

But by geometrical considerations, one can derive that, for a finite number N of paths the resonance in the vicinity an allowed energy level has width

$$\Delta E \approx \frac{nh^2}{\pi mNR^2},$$

where n is the index of the level. By substituting into the previous equation the previously derived expression for N , with the value $p=nh/R$ corresponding to an energy level, one finds $\Delta E \cdot \Delta t \approx \hbar$ independent of the energy level index.

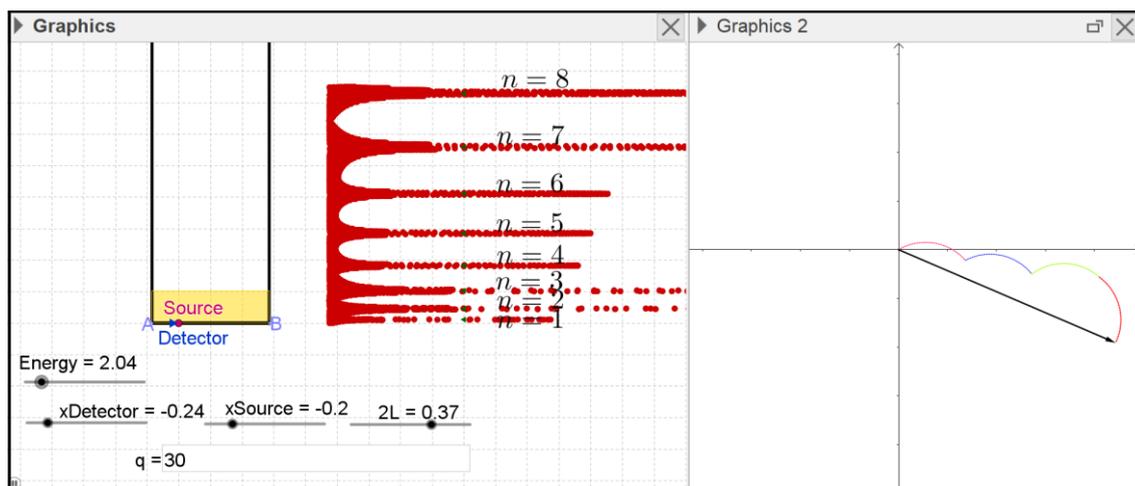


Figure 4 – Graph of the approximate spectrum of a particle-in-a-box system when only a finite number of paths (here $N = 120$ for all values of energy) is considered. The spread of spectral lines corresponding to energy levels into Lorentzian-like shapes is evident. The width of the peaks is not uniform because in this simulation N is kept fixed for all values of energy rather than depending on a fixed time uncertainty Δt and the particle momentum p .

It is rather straightforward to show that the same holds for the particle-in-a-box (see Figure 4), and indeed for all one-dimensional quantum systems, thus providing an important consistency check for the approach.

4. Five years of implementation

The educational reconstruction of quantum physics based on Feynman's approach can be the common base for teaching-learning sequences thought for different levels of instruction. We have so far performed experimentations:

- a) In the fourth year of Italian secondary school (17-18 year old students) limited to the quantum photon model and its relationship with the classical wave model [19]. For these experimentation the focus is on building an unified perspective of the different models for light (wave, ray, and quantum models) understanding the relationship between them, and the limits of validity.

- b) In the final year of secondary school (18-19 year old students), covering and extending the suggested material for the physics curriculum [20]. Here the attempt was to lead students integrated conceptual understanding of the "quantum object" model.
- c) With student teachers, both pre-service and in-service, and perspective teacher University students [18]. Within this setting, the most relevant problem is to have an approach that serves as an example on how to teach quantum theory (for physics students and graduates) but also is able to replace a standard university level course on quantum theory (for mathematics students and graduates).

5. Conclusions

In this work we discussed the features and possible implementations of teaching-learning sequences designed by our group and based on a time-independent, fixed energy sum over paths approach. We concentrated on describing how our approach can help students to analyze some typical problems in introductory quantum physics and to understand the relationship between energy and time, both in physics as a whole and in quantum physics in particular. Although the point of view of Feynman's sum over paths quantum theory is quite different from the one of the traditional Schrodinger formulation, the former may well constitute a complete and self-consistent educational reconstruction of quantum theory in its own right, bringing educational advantages and favoring conceptual understanding especially in the context of teaching in high school or to non-specialists.

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