Explicit Euler method for solving the time dependent Schrödinger equation

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Using an explicit Euler substitution, a system of differential equations was obtained, which can be used to find the solution of the time-dependent 1-dimensional Schrödinger equation for a general form of the time-dependent potential.

In the framework of fundamentals of Quantum mechanics, the unitary evolution given by the Schrödinger equation is conceivable only for quasi-isolated quantum systems, i.e. systems interacting via "classical" fields, which may be obtained using quantification procedures. Actually, these fields are time-independent, or have a harmonic time-dependence. The evolution of a quantum system interacting with a non-stationary environment is given by master-type equations rather than time-dependent Schrödinger equations. However, the latter are often used in many practical applications from molecular physics, quantum chemistry, quantum optics, solid state physics, etc. [1].

In the recent paper [1], I. Guedes obtained the exact Schrödinger wave function for a particle in a time-dependent 1-dimensional linear potential energy. For a Hamiltonian:

\[ H(x,p,t) = \frac{p^2}{2m} + f(t) \cdot x \]  

if Schrödinger equation is tested with the trial function:

\[ \Psi(x,t) = Ne^{[\eta(t) \cdot x + \mu(t)]} \]  

one obtains two differential equations for the functions \( \eta(t) \) and \( \mu(t) \), so one can find the solution \( \Psi(x,t) \) after solving these equations. To this end, one has to find the initial conditions, say from \( \Psi(x,0) \). However, \( \Psi(x,0) \) is not, generally, of the type [1], so one has to decompose \( \Psi(x,0) \) using Fourier series:

\[ \Psi(x,0) = \frac{1}{2\cdot\pi} \cdot \int_{-\infty}^{\infty} \tilde{\psi}(k) \cdot e^{-i k \cdot x} dk \]  

next find the initial conditions corresponding to the general component \( \tilde{\psi}(k) \cdot e^{-i k \cdot x} \), then one has to solve the differential equation for \( \eta(t,k) \) and \( \mu(t,k) \), and finally compute the inverse Fourier Transform.

Here I present an algorithm which can be used in solving the Schrödinger equation for a general form of the time and position dependence of potential energy, without referring to the Fourier Transform. One can test Schrödinger equation using the following explicit Euler substitution:

\[ \Psi(x,t) = N \cdot \exp[\sum_{n=0}^{\infty} \alpha_n(t) \cdot x^n] \]  

I used the series expansion of the potential energy w.r.t. \( x \):

\[ V(x,t) = \sum_{n=0}^{\infty} \frac{1}{n!} V_x^{(n)}(0,t) \cdot x^n \]  

The initial conditions are given by:

\[ \Psi(x,0) = N \cdot \exp[\sum_{n=0}^{\infty} \alpha_n(0) \cdot x^n] \]  

Expanding in power series, Schrödinger equation gives:

\[ \dot{\alpha}_n(t) - \frac{i \cdot \hbar}{2 \cdot m} [(n + 2) \cdot (n + 1) \cdot \alpha_{n+2} + \]

\[ + \sum_{k=0}^{n} (k+1) \cdot (n-k+1) \cdot \alpha_{k+1} \cdot \alpha_{n-k+1}] + \frac{1}{n!} V_x^{(n)}(0,t) = 0 \]

One can easily note that if one has non-zero initial coefficients only for \( n < n_0 \) (which includes \( \frac{1}{n!} V_x^{(n)}(0,t) \)), all coefficients for \( n < 2 \cdot n_0 \) have to remain zero at every subsequent moment (one can perform any-order time derivations in [2] at \( t = 0 \) and obtain null values). Relation [2] can be very useful, either for analytical calculations, or for numerical (finite difference) calculus algorithms:

\[ \alpha_{n+1} = \alpha_{n} + \frac{i \cdot \hbar}{2 \cdot m} [(n + 2) \cdot (n + 1) \cdot \alpha_{n+2} + \]

\[ + \sum_{k=0}^{n} (k+1) \cdot (n-k+1) \cdot \alpha_{k+1} \cdot \alpha_{n-k+1}] + \frac{1}{n!} V_x^{(n)}(0,p \cdot t_0) \]

In [3] a finite time step \( t_0 \) was chosen . It is obvious that one can iterate [3] in order to estimate \( \{\alpha_{n,p}\}_n \) for every moment \( p \cdot t_0 \) as functions of the initial coefficients \( \{\alpha_{n,0}\}_n \) given by [1].

[1] I. Guedes, Phys. Rev. A, 63, 034102 (2001).