

Transient phenomena in quantum mechanics

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Transient phenomena in quantum mechanics imply solving the time dependent Schrödinger equation with appropriate initial and boundary conditions. In this paper we consider the general formulation of the one dimensional problem and apply it to the particular example of transient phenomena for the bound state of a delta potential perturbed by the action of a boundary condition.

Keywords: Transient phenomena.

Fenómenos transitorios en mecánica cuántica implican resolver la ecuación de Schrödinger dependiente del tiempo con condiciones iniciales y de frontera. En este trabajo consideramos la formulación general del problema unidimensional y la aplicamos al ejemplo particular del fenómeno transitorio para el estado ligado de un potencial delta, perturbado por la acción de una condición a la frontera.

Descriptores: Fenómenos transitorios.

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1. Introduction

Bound states in quantum mechanics appear in many problems and, in particular, in the many electron systems of atoms. If the latter are suddenly subjected to the action of an electromagnetic or electrostatic field, transient phenomena occur. The mathematical formulation of the problem implies solving the time dependent Schrödinger equation for a given initial state, when we take into account the action of a suddenly applied external potential.

With present day computers these types of problems can be analyzed numerically in interesting physical situations such as that of an hydrogen atom in a suddenly applied electrostatic field. Yet before facing the just mentioned problem it is good to have a clear idea of what is its appropriate mathematical formulation, as well as discuss examples in which the analysis can be done analytically.

Thus in this note Sec. 2 deals with the general formulation of the problem in one dimension through the use of the Laplace transform, while Sec. 3 deals with a specific example.

In the conclusion we discuss the relevance of the ideas presented here to real physical situations.

2. The mathematical formulation of the problems

The ordinary time dependent one dimensional Schrödinger equation can be written as

$$\left[-i \frac{\partial}{\partial t} - \frac{1}{2} \frac{\partial^2}{\partial x^2} + V(x, t) \right] \psi(x, t) = 0 \quad (1)$$

where we use units in which \hbar and the mass m of the particle are 1.

The potential $V(x, t)$ changes suddenly at $t = 0$ i.e.

$$V(x, t) = \begin{cases} V_-(x) & \text{if } t < 0 \\ V_+(x) & \text{if } t > 0 \end{cases} \quad (2)$$

with $V_-(x)$ being of such type that it allows the possibility of bound states, while $V_+(x)$ has also added the effect of some external potential.

Our problem then is to find a solution of Eq. (1) for $t > 0$ with some initial condition

$$\psi(x, 0) = f(x) \quad (3)$$

where $f(x)$ is in turn a bound state satisfying

$$\left[-\frac{1}{2} \frac{d^2}{dx^2} + V_-(x) \right] f(x) = E_0 f(x) \quad (4)$$

for some given eigen energy $E_0 < 0$.

A general procedure for the analysis of these types of problems is to go through a Laplace transform of the wave function $\psi(x, t)$, which we designate by a bar above it as $\bar{\psi}(x, s)$, defined by

$$\bar{\psi}(x, s) = \mathcal{L}[\psi(x, t)] \equiv \int_0^\infty e^{-st} \psi(x, t) dt \quad (5)$$

with s being, in general, a complex number such that the integral exists. From (3) and (4) we see also that

$$\begin{aligned} \int_0^\infty e^{-st} \left[\frac{\partial \psi(x, t)}{\partial t} \right] dt &= \int_0^\infty \frac{\partial [e^{-st} \psi(x, t)]}{\partial t} dt + s \bar{\psi}(x, s) \\ &= -f(x) + s \bar{\psi}(x, s) \end{aligned} \quad (6)$$

assuming that s is in the region where $\exp(-st)$ tends to zero when $t \rightarrow \infty$.

Applying now a Laplace transform to Eq. (1) we see from (6) that it becomes

$$\left[-is - \frac{1}{2} \frac{d^2}{dx^2} + V_+(x) \right] \bar{\psi}(x, s) = -if(x) \quad (7)$$

where $V(x)$ is replaced by $V_+(x)$ as, in (5), t is in the interval $0 \leq t \leq \infty$.

Assuming that $\bar{\psi}(x, s)$ can be derived analytically we can obtain $\psi(x, t)$ through the inverse Laplace transform

$$\psi(x, t) = \mathcal{L}^{-1}[\bar{\psi}(x, s)] \equiv \frac{1}{2\pi i} \int_{c-i\infty}^{c+i\infty} e^{st} \bar{\psi}(x, s) ds \quad (8)$$

where c is a constant as indicated in Fig. 1 to the right of all possible singularities of $\bar{\psi}(x, s)$.

Sometimes it is convenient to change our variable s , and its corresponding contour, by introducing a new variable k through the definition

$$s = -ik^2/2 \quad (9)$$

so that the contour is modified to C' as indicated in Fig. 1 and thus we have

$$\begin{aligned} \psi(x, t) &= \mathcal{L}^{-1}[\bar{\psi}(x, k)] \\ &= -\frac{1}{2\pi} \int_{C'} e^{-ik^2 t/2} \bar{\psi}(x, k) k dk \end{aligned} \quad (10)$$

where we use the more compact notation

$$\bar{\psi}(x, -ik^2/2) \rightarrow \bar{\psi}(x, k). \quad (11)$$

We can complete the contour C' with the dotted semicircle because on it $\exp(-ik^2 t/2) \rightarrow 0$ when $|k| \rightarrow \infty$. As the integral is an analytic function we can deform the contour to that of C'' on the real axis, also indicated in Fig. 1, and we have the result on k -space

$$\begin{aligned} \psi(x, t) &= -\frac{1}{2\pi} \int_{-\infty}^{\infty} e^{-ik^2 t/2} \bar{\psi}(x, k) k dk \\ &+ i \sum_n \text{Res} \left[e^{-ik^2 t/2} \bar{\psi}(x, k) k, k_n \right], \end{aligned} \quad (12)$$

where the integral is done raising the contour around any pole on the real axis, and the residues correspond to the poles k_n in the upper half plane.

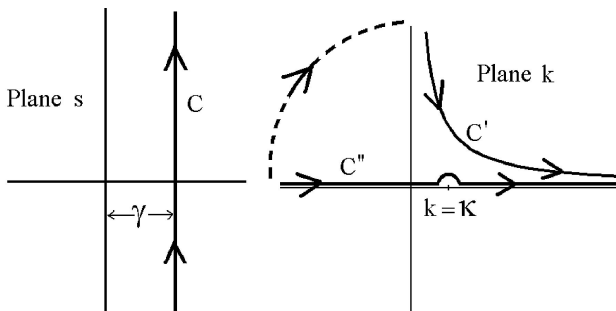


FIGURE 1. Inverse Laplace transform integration path, in plane s and in plane k .

From (7) we see that $\bar{\psi}(x, k)$ satisfies now the equation

$$\left[\frac{d^2}{dx^2} + k^2 - 2V_+(x) \right] \bar{\psi}(x, k) = 2if(x) \quad (13)$$

which, in general, is quite difficult to solve.

We shall see though, in the next section, a case in which it can be determined analytically.

3. Discussion of an analytic example

We shall consider a one dimensional potential $V(x, t)$ for which

$$V_-(x) = -A\delta(x),$$

$$V_+(x) = -A\delta(x) + B\delta(x-b) + B\delta(x+b) \quad (14)$$

where A, B, b are positive real constants. Next we take the limit $B \rightarrow \infty$, so we can have reflecting walls at $x = \pm b$.

For negative times, from Eq. (4), the bound state $f(x)$ satisfies the equation

$$\left[-\frac{1}{2} \frac{d^2}{dx^2} - A\delta(x) \right] f(x) = -\frac{\lambda^2}{2} f(x) \quad (15)$$

where the negative energy E_0 is replaced by $-(\lambda^2/2)$. The normalized eigen solution of Eq. (15) is a well known result reported in standard books of Quantum Mechanics [1] and is given by

$$f(x) = A^{1/2} \exp[-A|x|], \quad \lambda = A. \quad (16)$$

For positive times, from Eq. (13) we see that the Laplace transform $\bar{\psi}(x, k)$ of our wave function $\psi(x, t)$ satisfies the equation

$$\begin{aligned} \left[\frac{d^2}{dx^2} + k^2 + 2A\delta(x) \right] \bar{\psi}(x, k) \\ = 2iA^{1/2} \exp(-A|x|), \end{aligned} \quad (17)$$

defined in the range $-b \leq x \leq b$, with boundary conditions: $\bar{\psi}(b, k) = \bar{\psi}(-b, k) = 0$. Notice that since the potential and the initial condition are symmetric functions of x , the time dependent solution must also have even parity at all times $\psi(-x, t) = \psi(x, t)$.

For $x \neq 0$, we have the simpler equation

$$\left[\frac{d^2}{dx^2} + k^2 \right] \bar{\psi}(x, k) = 2iA^{1/2} \exp(-A|x|), \quad (18)$$

which has the general symmetric solution ($\bar{\psi}_+$, $\bar{\psi}_-$) at the right and left of the delta singularity at $x = 0$,

$$\begin{aligned} \bar{\psi}_+(x, k) &= C \exp(ikx) + D \exp(-ikx) \\ &+ \frac{2iA^{1/2} \exp(-Ax)}{k^2 + A^2} \end{aligned} \quad (19)$$

$$\begin{aligned} \bar{\psi}_-(x, k) &= D \exp(ikx) + C \exp(-ikx) \\ &+ \frac{2iA^{1/2} \exp(+Ax)}{k^2 + A^2} \end{aligned} \quad (20)$$

The constants $C(s)$ and $D(s)$ are determined by two conditions: 1) discontinuity at $x = 0$ of the first derivative

$$\lim_{\epsilon \rightarrow 0} \left[\frac{d\bar{\psi}_+(\epsilon, k)}{dx} - \frac{d\bar{\psi}_-(-\epsilon, k)}{dx} \right] + 2A\bar{\psi}_+(0, k) = 0 \quad (21)$$

and 2) the boundary condition at $x = b$

$$\bar{\psi}_+(b, k) = 0. \quad (22)$$

The symmetry of the solution assures that the two additional conditions: 3) continuity of $\bar{\psi}$ at $x = 0$ and 4) the boundary condition $\bar{\psi}_-(-b, s) = 0$, are automatically satisfied.

Eqs. (21) and (22) lead to the relations

$$\begin{pmatrix} A + ik & A - ik \\ \exp(ikb) & \exp(-ikb) \end{pmatrix} \begin{pmatrix} C \\ D \end{pmatrix} = \begin{pmatrix} 0 \\ -2i\sqrt{A} \exp(-Ab)/(k^2 + A^2) \end{pmatrix} \quad (23)$$

with a solution given by

$$C(k) = \frac{A^{1/2} \exp(-Ab)}{(A + ik)(k \cos kb - A \sin kb)}, \quad (24)$$

$$D(k) = \frac{-A^{1/2} \exp(-Ab)}{(A - ik)(k \cos kb - A \sin kb)}. \quad (25)$$

Therefore we have the complete and exact solution for the wave function in k -space as

$$\begin{aligned} \bar{\psi}_+(x, k) &= \frac{-iA^{1/2} \exp(-Ab)}{(k \cos kb - A \sin kb)} \\ &\times \left[\frac{\exp(ikx)}{(k - iA)} + \frac{\exp(-ikx)}{(k + iA)} \right] + \frac{2iA^{1/2} \exp(-Ax)}{k^2 + A^2} \end{aligned} \quad (26)$$

$$\bar{\psi}_-(x, k) = \bar{\psi}_+(-x, k) \quad (27)$$

Consider now the inverse Laplace transform of Eq. (26). The inverse transform of the stationary state contribution (the last term) can be done immediately

$$\begin{aligned} \mathcal{L}^{-1} \left[\frac{2iA^{1/2} \exp(-Ax)}{k^2 + A^2} \right] \\ = A^{1/2} \exp(-Ax) \exp(iA^2 t/2). \end{aligned} \quad (28)$$

which, as expected, is just the initial bound state with a phase $-i\epsilon t/\hbar \rightarrow +A^2 t/2$.

As for the inverse of the transient part (the first two terms in Eq. (26)) consider for instance

$$\mathcal{L}^{-1} \left[\frac{kb}{(kb \cos kb - Ab \sin kb)} \frac{\exp(ikx)}{k(k - iA)} \right]. \quad (29)$$

Notice that we have inserted a factor kb in the numerator (which cancels out with a similar term in the denominator) in anticipation of things to come. The main problem now is that for $z \equiv kb$ the function of a complex variable $f(z)$ defined by

$$f(z) \equiv \frac{z}{z \cos z - Ab \sin z}, \quad (30)$$

yields an infinite number of poles at $z = z_j$ given by the roots of the transcendental equation, see Fig. 2

$$\tan z_j = z_j / Ab. \quad (31)$$

However, since the meromorphic function $f(z)$ has poles $z_j \neq 0$ (the origin is a removable singularity) which can be classified by magnitude

$$0 < |z_1| \leq |z_2| \leq \dots \leq |z_j| \leq \dots, \quad (32)$$

and each pole has a corresponding residues $r_j = z_j / [(1 - Ab) \cos z_j - z_j \sin z_j]$, then we can write a Mittag-Leffler expansion [2]

$$f(z) = f(0) + \sum_{j=1}^{\infty} r_j \left(\frac{1}{z - z_j} + \frac{1}{z_j} \right), \quad (33)$$

with $f(0) = (1 - Ab)^{-1}$. Therefore Eq. (29) becomes

$$\begin{aligned} \mathcal{L}^{-1} \left[f(kb) \frac{\exp(ikx)}{k(k - iA)} \right] \\ = \mathcal{L}^{-1} \left[\left\{ f(0) + \sum_{j=1}^{\infty} \left(\frac{r_j}{kb - z_j} + \frac{r_j}{z_j} \right) \right\} \frac{\exp(ikx)}{k(k - iA)} \right] \end{aligned} \quad (34)$$

An now the inversion can be easily carried out in terms of the diffraction in time[3] function $M(x, \kappa, t)$ defined in terms of the complementary error function

$$\begin{aligned} M(x, \kappa, t) &\equiv \mathcal{L}^{-1} \left[\frac{\exp(ikx)}{ik(k - \kappa)} \right] \\ &= -\frac{1}{2\pi i} \int_{-\infty}^{\infty} \exp(-ik^2 t/2) \frac{\exp(ikx)}{k - \kappa} dk \\ &= \frac{1}{2} \exp(ikx - i\kappa^2 t/2) \operatorname{erfc} \left[\frac{(x - \kappa t)}{(2it)^{1/2}} \right]. \end{aligned} \quad (35)$$

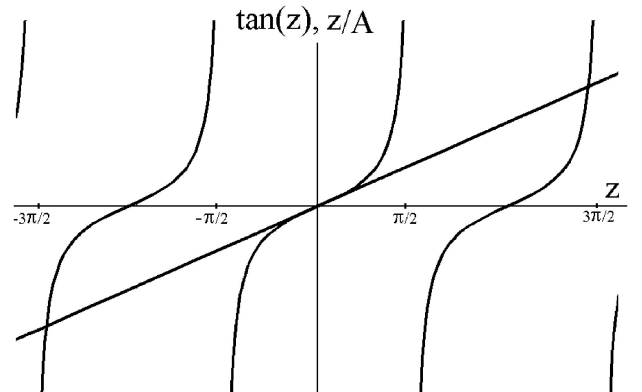


FIGURE 2. Plot of $\{\tan(z), z/Ab\}$, showing the infinite number of roots of the equation $\tan z = z/Ab$.

Finally, for the exact analytic wave function we have

$$\begin{aligned}
 \psi_+(x, t) &= \mathcal{L}^{-1} \left[C(k)e^{ikx} + D(k)e^{-ikx} + \frac{2iA^{1/2} \exp(-Ax)}{k^2 + A^2} \right] \\
 &= \left[A^{1/2} e^{-Ab} \left[\left\{ f(0) + \sum_{j=1}^{\infty} \left(\frac{r_j}{z_j} - \frac{r_j}{z_j - iAb} \right) \right\} M(x, iA, t) + \sum_{j=1}^{\infty} \frac{ir_j}{z_j - iAb} M(x, z_j/b, t) \right] \right. \\
 &\quad \left. + \left[A^{1/2} e^{-Ab} \left[\left\{ f(0) + \sum_{j=1}^{\infty} \left(\frac{r_j}{z_j} - \frac{r_j}{z_j + iAb} \right) \right\} M(-x, -iA, t) + \sum_{j=1}^{\infty} \frac{ir_j}{z_j + iAb} M(-x, z_j/b, t) \right] \right] \right. \\
 &\quad \left. + A^{1/2} \exp(-Ax) \exp(iA^2 t/2) \right] \quad (36)
 \end{aligned}$$

with $f(0) = (1 - Ab)^{-1}$ as given before Eq. (34). Note that

$$\psi_-(x, t) = \psi_+(-x, t). \quad (37)$$

4. Conclusion

The problem we discussed has the advantage that it can be solved analytically using only the wave function $M(x, \kappa, t)$ that appear in the old problem of diffraction in time [3].

With the help of the Mittag-Leffler development this result probably would still be valid for more physical cases in which an electrostatic field is suddenly applied to bound states of electrons in atoms or nucleons in nuclei.

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1. W. Greiner, *Quantum Mechanics*, (Springer-Verlag, Berlin, 1994), pag. 115.
2. P. Dennery and A. Krzywicki, *Mathematics for Physicist*, (Harper and Row, New York 1967), pag 84, Eq. (29.5).
3. M. Moshinsky, *Phys. Rev.* **88**, 625 (1952).