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Comparison between perturbative and exact transitions induced by an interaction

M. Moshinsky*, G. Loyola and C. Villegas

Instituto de Física, Universidad Nacional Autónoma de México
Apartado postal 20-364, 01000 México, D.F., México

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Abstract. When discussing time dependent perturbation theory in quantum mechanics, students occasionally ask whether there are time dependent Schrödinger equations that can be solved exactly. They then suggest that this would allow a comparison between exact and perturbative transitions between energy states induced by an interaction. In this paper we implement this program for a Hamiltonian in a one dimensional space consisting of the kinetic energy plus a delta function interaction. The exact solutions were obtained with the help of those developed long ago for the problem of diffraction in time and, as expected, they give the perturbative result for large times and weak interactions. In the final section we indicate that the validity of our conclusions is more general than the simple example that illustrates them in this paper.

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1. Introduction

Among the subjects in a course on quantum mechanics the discussion of transitions between energy levels induced by an interaction occupies an important place. One of the approaches to this subject [1] is through time dependent perturbation theory, which is an approximate solution to the Schrödinger equation

$$i\hbar\frac{\partial\psi}{\partial t} = (H_0 + U)\psi, \tag{1.1}$$

where t is the time in the usual units and H_0 is a Hamiltonian with well known eigenvalues E_n and orthonormal eigenfuctions $\varphi_n(x)$, and U is the interaction causing the transitions. Proposing a solution of the form [1]

$$\psi = \sum_n a_n(t)\varphi_n(x)\exp(-iE_nt/\hbar) \tag{1.2}$$

*Member of El Colegio Nacional.

the a_n satisfy the infinite set of first order ordinary differential equations

$$i\hbar\dot{a}_{n''}(t) = \sum_n \langle n''|U|n\rangle a_n(t)\exp\left[-i\hbar^{-1}(E_n - E_{n''})t\right] \tag{1.3a}$$

with the initial condition

$$a_n(0) = \delta_{nn'}. \tag{1.3b}$$

The exact solution of (1.3) is just as difficult as that of (1.1), but the first order perturbative approach, based on the substitution of $a_n(t)$ by $\delta_{nn'}$ in the right hand side of (1.3a) is trivial, giving [1]

$$a_{n''}(t) = (E_{n'} - E_{n''})^{-1}\left[\exp[-i(E_{n'} - E_{n''})t\hbar^{-1}] - 1\right]\langle n''|U|n'\rangle. \tag{1.4}$$

From this result follows the standard discussion [1] that relates the probability of transition per unit time with $|\langle n''|U|n'\rangle|^2$.

When the above analysis is presented, an occasionally perceptive student asks whether there are not examples in which the ψ of (1.1) or, equivalently, the $a_n(t)$ of (1.3), can be determined exactly and the result compared with (1.4). Of course today we can use a computer to solve (1.1) numerically, but as Wigner once observed when presented with results of this type "it is nice to know that the computer understands the problem, but I would like to understand it too". Thus a discussion of a simple case in which the solution of (1.1) can be found analytically seems of some interest, and we will proceed to do this in the present paper.

2. The problem

We shall consider Eq. (1.1) in one space dimension with H_0 being just the kinetic energy operator and U a δ function interaction, *i.e.*

$$i\hbar\frac{\partial\psi}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2} + V_0\delta\left(\frac{x}{a}\right)\psi, \tag{2.1}$$

where a will be taken as the Bohr radius $a = (\hbar^2/me^2)$ and x, t are given in centimeters and seconds respectively. In atomic units $e = \hbar = m = 1$ we have *dimensionless* x, t in terms of which Eq. (2.1) becomes

$$i\frac{\partial\psi}{\partial t} = -\frac{1}{2}\frac{\partial^2\psi}{\partial x^2} + b\delta(x)\psi, \tag{2.2}$$

where $b = (me^4/\hbar^2)^{-1}V_0$.

For a perturbation analysis along the lines of the previous section, it is convenient to enclose the problem in a linear box going from $x = -\ell$ to $x = \ell$ and impose periodic boundary conditions in the extremes. The orthonormal eigenfunctions $\varphi_n(x)$ of H_0 are then

$$\varphi_n(x) = (2\ell)^{-1/2} \exp(in\pi x/\ell), \tag{2.3}$$

while the eigenvalues for energy and momentum are respectively

$$E_n = \frac{1}{2}\left(\frac{n\pi}{\ell}\right)^2, \qquad p_n = \left(\frac{n\pi}{\ell}\right). \tag{2.4a, b}$$

The matrix element of $U(x) = b\delta(x)$ is then

$$\langle n''|U|n'\rangle = (2\ell)^{-1}b, \tag{2.5}$$

and thus, with the initial condition $a_n(0) = \delta_{nn'}$, we have from (1.4) that

$$|a_{n''}(t)|^2 = (2\ell)^{-2}b^2 \frac{\sin^2[(E_{n'} - E_{n''})t/2]}{[(E_{n'} - E_{n''})/2]^2}. \tag{2.6}$$

We can replace E_n by p_n in this equation and using the short hand notation

$$p' \equiv \frac{n'\pi}{\ell}, \quad p'' = \frac{n''\pi}{\ell}, \tag{2.7}$$

the expression on the right hand side of (2.6) can be written as

$$(2\ell)^{-2}b^2 \left[\frac{1}{4}(p'^2 - p''^2)\right]^{-2} \sin^2\left[\frac{1}{4}(p'^2 - p''^2)t\right], \tag{2.8}$$

which will be the perturbative result for the problem.

In the exact case, we choose as initial condition a wave-function of momentum p' in the full interval $-\infty \leq x \leq \infty$, normalized in the Dirac delta sense, so we are looking for a solution $\psi(x, p', t)$ of (2.2) with the initial value

$$\psi(x, p', 0) = (2\pi)^{-1/2} \exp(ip'x). \tag{2.9}$$

Once we obtain $\psi(x, p', t)$ we shall determine its scalar product with a wavefunction of momentum p'', *i.e.*

$$\int_{-\infty}^{\infty} (2\pi)^{-1/2} \exp(-ip''x)\psi(x, p', t)dx \equiv g(p'', p', t), \tag{2.10}$$

and consider the conditions for which a meaningful comparison can be made between

$$|g(p'', p', t)|^2 \tag{2.11}$$

and the expression (2.8).

To implement our program we first need to determine explicitly $\psi(x, p', t)$ satisfying (2.2) and (2.9), which we shall proceed to do in the next section.

3. Determination of $\psi(x, p', t)$

To determine the solution of a time dependent equation with a given initial value, the obvious procedure is to use the Laplace transform [2]

$$\bar{\psi}(x, p', s) = \int_0^\infty \psi(x, p', t) e^{-st} dt. \tag{3.1}$$

Applying it to both sides of equation (2.2) we get

$$-i\psi(x, p', 0) + is\bar{\psi}(x, p', s) = \left[-\frac{1}{2}\frac{d^2}{dx^2} + b\delta(x)\right] \bar{\psi}(x, p', s). \tag{3.2}$$

We consider first the case when $x \neq 0$ so the δ function does not appear and using the initial condition (2.9) we have

$$-i\frac{e^{ip'x}}{\sqrt{2\pi}} = \left(-\frac{1}{2}\frac{d^2}{dx^2} - is\right) \bar{\psi}(x, p', s), \tag{3.3}$$

for which we can propose the solution

$$\bar{\psi}(x, p', s) = A \exp\left[i(2is)^{1/2}|x|\right] + B \exp(ip'x) \tag{3.4}$$

where A, B are so far undetermined constants.

We note that $\exp[\pm i(2is)^{1/2}x]$ satisfies the homogeneous equation obtained when the right hand side of (3.3) is equated to 0. Our choice of

$$\exp\left[i(2is)^{1/2}|x|\right] = \exp\left[(i-1)s^{1/2}|x|\right], \tag{3.5}$$

is due to the fact that we consider $s > 0$ and when $x > 0$, *i.e.* $|x| = x$ and $x \to +\infty$, the exponential vanishes, as is also the case when $x < 0$, *i.e.* $|x| = -x$ and $x \to -\infty$.

Thus (3.4) is a bounded solution of (3.3) if we choose

$$B = -\frac{i}{(2\pi)^{1/2}}\left(\frac{1}{2}p'^2 - is\right)^{-1} \tag{3.6}$$

while A still remains arbitrary.

We note that the function (3.4) is continuous at $x = 0$, but does not have a continuous derivative at this point due to the appearance of the absolute value $|x|$ in one of the exponentials. The value of the discontinuity can be determined by integrating with respect to x, between $-\epsilon$ and ϵ, on both sides of Eq. (3.2) and take the limit $\epsilon \to 0$. We thus obtain the relation

$$-\frac{1}{2}\left\{\left[\frac{d\bar{\psi}(x,p',s)}{dx}\right]_{x=+0} - \left[\frac{d\bar{\psi}(x,p',s)}{dx}\right]_{x=-0}\right\} + b\bar{\psi}(0,p',s) = 0, \tag{3.7}$$

which leads to the equation

$$(b - i\sqrt{2is})A + bB = 0 \tag{3.8}$$

that determines A. Thus finally we have

$$\bar{\psi}(x,p',s) = \frac{1}{\sqrt{2\pi}}\left\{\frac{e^{ip'x}}{(s + i\frac{p'^2}{2})} + \frac{2b\; e^{i(2is)^{1/2}|x|}}{(2is - p'^2)[(2is)^{1/2} + ib]}\right\}. \tag{3.9}$$

The function $\psi(x,p',t)$ is then obtained from $\bar{\psi}(x,p',s)$ by the inverse Laplace transform over the Bromwhich contour [2]

$$\psi(x,p',t) = \frac{1}{2\pi i}\int_{c-i\infty}^{c+i\infty} \bar{\psi}(x,p',s)e^{st}ds, \tag{3.10}$$

where c is a positive constant that puts the integration line parallel to the imaginary axis of the s-plane but to the right of any poles or branch points of the function $\bar{\psi}(x,p',s)$ of s.

Using the explicit expression (3.9) of $\bar{\psi}(x,p',s)$, the integration of the part in $e^{ip'x}$ is immediate and thus we have

$$\psi(x,p',t) = \frac{1}{\sqrt{2\pi}}\left\{e^{i(p'x - \frac{1}{2}p'^2t)} + \frac{1}{2\pi i}\int_{c-i\infty}^{c+i\infty}\frac{(2b)e^{i(2is)^{1/2}|x|}e^{st}ds}{(2is - p'^2)[(2is)^{1/2} + ib]}\right\}. \tag{3.11}$$

We now multiply numerator and denominator in the integral in (3.11) by $(2is)^{1/2}$ and introducing the notation

$$(2is)^{1/2} \equiv z, \tag{3.12}$$

we consider the expression

$$\frac{z}{(z-p')(z+p')(z+ib)} = \frac{1}{2(p'+ib)(z-p')} - \frac{1}{2(p'-ib)(z+p')} + \frac{ib}{(p'^2+b^2)(z+ib)} \tag{3.13}$$

where the right hand side is obtained from the theory of residues [3].

Substituting (3.13) in (3.11) we see that the integrals we have to evaluate are all of the form

$$\frac{1}{2\pi i}\int_{c-i\infty}^{c+i\infty} \frac{e^{i(2is)^{1/2}|x|}e^{st}ds}{\sqrt{2is}(\sqrt{2is}-k)} = -\frac{i}{2}\chi(|x|,k,t), \tag{3.14}$$

where $k = p', -p'$ or $-ib$ and, as shown in the Appendix and in Ref. [4], the functional form of $\chi(|x|,k,t)$ is

$$\chi(|x|,k,t) = e^{i(x^2/2t)}e^{y^2}\operatorname{erfc}(y), \tag{3.15}$$

where

$$y = e^{-i\pi/4}(2t)^{-1/2}(|x|-kt), \tag{3.16}$$

and

$$\operatorname{erfc}(y) = \frac{2}{\sqrt{\pi}}\int_y^\infty e^{-z^2}dz \tag{3.17}$$

is the error integral function.

Thus the $\psi(x,p',t)$ satisfying the equation (2.2) and initial condition (2.9) has the explicit form

$$\begin{aligned}\psi(x,p',t) = \frac{1}{(2\pi)^{1/2}}\bigg\{&\exp[i(p'x-\frac{1}{2}p'^2t)] - \frac{ib}{2(p'+ib)}\chi(|x|,p',t)\\ &+\frac{ib}{2(p'-ib)}\chi(|x|,-p',t) + \frac{b^2}{p'^2+b^2}\chi(|x|,-ib,t)\bigg\}.\end{aligned} \tag{3.18}$$

We now check directly that $\psi(x,p',t)$ satisfies all our requirements. First we note that [4]

$$i\frac{\partial\chi}{\partial t} + \frac{1}{2}\frac{\partial^2\chi}{\partial x^2} = (4it)^{-1}\exp(ix^2/2t)\left\{\left[\frac{d^2}{dy^2} - 2y\frac{d}{dy} - 2\right]\exp(y^2)\operatorname{erfc}(y)\right\} = 0, \tag{3.19}$$

and thus for $x \neq 0$ the equation

$$i\frac{\partial\psi(x,p',t)}{\partial t} = -\frac{1}{2}\frac{\partial^2\psi(x,p',t)}{\partial x^2} \tag{3.20}$$

is satisfied. The ψ is continuous at $x = 0$, and the presence of the δ function there implies, by the same reasoning as the one leading to (3.7), that

$$-\frac{1}{2}\left\{\left[\frac{\partial\psi(x,p',t)}{\partial x}\right]_{x=+0}-\left[\frac{\partial\psi(x,p',t)}{\partial x}\right]_{x=-0}\right\}+b\psi(0,p',t)=0. \tag{3.21}$$

From the fact that

$$\begin{aligned}\left[\frac{\partial\chi(x,k,t)}{\partial x}\right]_{x=0}&=\left\{\left[\frac{d}{dy}e^{y^2}\operatorname{erfc}(y)\right]\frac{\partial y}{\partial x}\right\}_{x=0}\\&=-(2/\pi t)^{1/2}e^{-i\pi/4}+ik\chi(0,k,t),\end{aligned} \tag{3.22}$$

we easily check that Eq. (3.21) is satisfied, so that $\psi(x,p',t)$ is a solution of (2.2).

Besides, when $|y|\to\infty$ we have that [4]

$$e^{y^2}\operatorname{erfc}(y)\to\begin{cases}0 & \text{if } -(\pi/2)<\arg y<\pi/2\\ 2e^{y^2} & \text{if } (\pi/2)<\arg y<3\pi/2.\end{cases} \tag{3.23}$$

When $t\to 0, y\to e^{-i\pi/4}(2t)^{-1/2}x\to e^{-i\pi/4}\infty$, so $\arg y=-(\pi/4)$ and $\chi(|x|,k,t)\to 0$ implying that the initial condition (2.9) is satisfied.

Thus we have checked that $\psi(x,p',t)$ given by (3.18) satisfies the equation (2.2) and the initial condition (2.9). The next question is to obtain the $g(p'',p',t)$ defined by (2.10), which we proceed to do in the following section.

4. Determination of $g(p'',p',t)$

Dividing the interval $-\infty\le x\le\infty$ into $-\infty\le x\le 0$ and $0\le x\le\infty$, the $g(p'',p',t)$ of (2.10) can be written as

$$g(p'',p',t)=\frac{1}{(2\pi)^{1/2}}\left[\int_0^\infty e^{-ip''x}\psi(x,p',t)dx+\int_0^\infty e^{ip''x}\psi(-x,p',t)dx\right] \tag{4.1}$$

which implies that the only integral we need to evaluate is

$$\int_0^\infty e^{\pm ip''x}\chi(|x|,k,t)dx=\frac{i}{(k\pm p'')}\Big[\chi(0,k,t)-\chi(0,\mp p'',t)\Big], \tag{4.2}$$

where the right hand side is a result obtained in the Appendix of Ref. [5]. From (3.15) we see that for $x=0$

$$\chi(0,k,t)=e^{u^2}\operatorname{erfc}(u) \tag{4.3a}$$

with

$$u = -e^{-i\pi/4}k(t/2)^{1/2}. \tag{4.3b}$$

Making use of (4.2) and grouping together the coefficients of $\chi(0,k,t)$ where $k = \pm p', \pm p''$ or $-ib$, we obtain

$$\begin{aligned} g(p'',p',t) = \delta(p'-p'')e^{-i\frac{1}{2}p'^2 t} + \frac{1}{2\pi}\left\{\frac{p'b}{(p'+ib)}\frac{\chi(0,p',t)}{(p'^2-p''^2)}\right. \\ + \frac{p'b}{(p'-ib)}\frac{\chi(0,-p',t)}{(p'^2-p''^2)} + \frac{p''b}{(p''+ib)}\frac{\chi(0,p'',t)}{(p''^2-p'^2)} \\ \left. + \frac{p''b}{(p''-ib)}\frac{\chi(0,-p'',t)}{(p''^2-p'^2)} - \frac{2b^3}{(p'^2+b^2)}\frac{\chi(0,-ib,t)}{(p''^2+b^2)}\right\}. \end{aligned} \tag{4.4}$$

Thus we have an exact analytic expression for $g(p'',p',t)$, as $\chi(0,k,t)$ is given by (4.3).

We proceed now to compare $|g(p'',p',t)|^2$ with the result (2.8) of the perturbative approach, as well as to give an explicit series expression for $g(p'',p',t)$ in terms of powers of $t^{1/2}$.

5. Comparison between perturbative and exact transitions induced by an interaction

As mentioned in the discussion of time dependent perturbations [1], the physically relevant result is obtained when one considers times t large as compared to $(\hbar/E)$ where E are the energies involved. In the units used here this implies $(k^2t/2) \gg 1$ for $k = \pm p', \pm p''$ or $-ib$, so that $|u|$ in (4.3b) tends to ∞. In this case we can replace $\exp u^2 \operatorname{erfc}(u)$ by its asymptotic value, and using (3.23) we see that

$$\chi(0,p',t) \to 2\exp(-ip'^2t/2), \quad \chi(0,p'',t) \to 2\exp(-ip''^2t/2), \tag{5.1}$$

while all the other $\chi(0,k,t), k = -p', -p'', -ib$ vanish. Thus, for $p' \neq p''$, we are left with

$$\begin{aligned} g(p'',p',t) &\simeq \frac{1}{\pi}\left\{\frac{p'b\exp(-ip'^2t/2)}{(p'+ib)(p'^2-p''^2)} + \frac{p''b\exp(-ip''^2t/2)}{(p''+ib)(p''^2-p'^2)}\right\} \\ &= \frac{b}{\pi}\left\{\left[\frac{\exp(-ip'^2t/2)-\exp(-ip''^2t/2)}{(p'^2-p''^2)}\right]\right. \\ &\quad \left. - \left[\frac{ib}{(p'+ib)}\exp(-ip'^2t/2) - \frac{ib}{(p''+ib)}\exp(-ip''^2t/2)\right]\frac{1}{p'^2-p''^2}\right\}. \end{aligned} \tag{5.2}$$

If we further assume that $b \ll p', p''$, which would be the natural restriction for the validity of a perturbation approximation, *i.e.* that the strength of the interaction is much smaller than the kinetic energy of the particle, we are left with

$$g(p'', p', t) \simeq \frac{b}{\pi}\left(\frac{e^{-i\frac{1}{2}p'^2 t} - e^{-i\frac{1}{2}p''^2 t}}{p'^2 - p''^2}\right) \tag{5.3}$$

when $|k|t \gg 1$ for $|k| = |p'|, |p''|$ or b, and $b \ll |p'|$ or $|p''|$.

The squared absolute value of $g(p'', p', t)$ is then

$$|g(p'', p', t)|^2 = \frac{b^2}{(2\pi)^2}\frac{\sin^2\left[\frac{1}{4}(p'^2 - p''^2)t\right]}{\left[\frac{1}{4}(p'^2 - p''^2)\right]^2}, \tag{5.4}$$

which coincides with the perturbative value (2.8) except for the fact that instead of $(2\ell)^{-2}$ in the latter we have $(2\pi)^{-2}$ in (5.4) due to the different types of normalization we chose in the two cases.

The exact solution for transitions due to an interaction goes into the perturbative one when the conditions mentioned after (5.2) are satisfied. New results will come out though if $|k|t$ is of order or smaller than 1 for $|k| = |p'|, |p''|$ or b. In this case it is better to express $\chi(0, k, t)$ as a series in powers of the u of (4.3*b*), *i.e.*

$$\chi(0, k, t) = e^{u^2}\left(1 - \frac{2}{\sqrt{\pi}}\int_0^u e^{-z^2}dz\right) = \sum_{r=0}^{\infty} a_r u^r \tag{5.5}$$

where writing e^{u^2}, e^{-z^2}, as power series we arrive at the values

$$a_{2r} = \frac{1}{r!}, \quad a_{2r+1} = -\frac{2}{\sqrt{\pi}}\sum_{n=0}^{r}\frac{(-1)^n}{(r-n)!n!(2n+1)}. \tag{5.6}$$

Using then the developments (4.4), (5.5) and the explicit form (4.3*b*) for u, we get for $p' \neq p''$ that

$$g(p'', p', t) = \frac{1}{2\pi}\sum_{r=0}^{\infty}\left\{\left[a_{2r} + a_{2r+1}be^{i\pi/4}(t/2)^{1/2}\right]\frac{(-it/2)^r 2b}{(p'^2 - p''^2)}\right.$$
$$\left.\times\left[\frac{p'^{2r+2}}{p'^2 + b^2} - \frac{p''^{2r+2}}{p''^2 + b^2} - \frac{(p'^2 - p''^2)(-1)^r b^{2r+2}}{(p'^2 + b^2)(p''^2 + b^2)}\right]\right\}. \tag{5.7}$$

We easily check that the time independent term is 0, as it should be, because the initial value is $g(p'', p', 0) = \delta(p'' - p')$, which vanishes for $p' \neq p''$. For the term proportional to $t^{1/2}$ the coefficient happens also to vanish, so the first contribution is linear in t and if we calculate it we obtain

$$\frac{-ibt}{2\pi}, \tag{5.8}$$

so for very short times, *i.e.* $|k^2|t \ll 1$ for $|k| = |p'|, |p''|, b$, the probability of transition from p' to p'' due to the interaction is proportional to t^2.

In the concluding section we discuss some generalizations and possible applications of our present analysis.

6. Conclusion

In the example discussed in this paper, the interaction causing the transition is a very simple one, *i.e.* $b\delta(x)$. One could ask whether a similar analysis can be carried out for an arbitrary short range potential in three dimensions.

Actually this was done long ago [6], showing that if the initial wave function was *outside* the range r_0 of the potential, the scattered one, also for $r > r_0$, could be expressed in terms of the functions $r^{-1}\chi(r,k,t)$, where now k, besides $\pm p'$, takes the values at the poles of the S matrix of the problem, that appear only in the lower part or on the imaginary axis of the wave number plane.

Unfortunately, the time dependent state can not be determined explicitly and analytically *inside* the arbitrary short range potential, and thus its Fourier transform, *i.e.* the expression equivalent to $g(p'', p', t)$ in this paper, can not be obtained, so a comparison with the perturbative approach is not feasible. Thus the reason for the simple example discussed in this paper.

There is a case in which the time dependent solution for an interaction process can be obtained exactly. This corresponds [7] to a schematic theory of interactions in Fock space through boundary conditions at the point of coincidence of the particles, and where the resulting cross section is given by the Breit-Wigner formula [7].

In this case, the solution depends on $r^{-1}\chi(r,k,t)$ in the full interval $0 \le r \le \infty$ and k, besides the values $\pm p'$, also takes one of the single poles of the S matrix [8]. The Fourier transform of the state [9] is feasible and thus also the comparison with the perturbative approximation. In fact, the problem is very similar to that of $\psi(x, p', t)$ in (3.18) and $g(p'', p', t)$ in (4.4), with the $-ib$, appearing in $\chi(|x|, -ib, t)$, being replaced by the complex pole k_0 of the S matrix.

Clearly then the exact transitions caused by an interaction go quite generally into the perturbative ones, when $|k|t \gg 1$ and the strength of the interaction is small compared with the energy of ingoing and outgoing particles, as we should expect.

We note also that through (5.7) we can calculate the probability of transition between p' and p'', by means of a series in powers of $t^{1/2}$, and thus we can analyze situations in which the interaction is operating during very short times, which seems to be occurring quite frequently in present day experiments.

Finally, we remark that all the above examples are non relativistic. We have discussed though the problem of diffraction in time for the Dirac equation [10], and thus we are in a position to analyze the one dimensional Dirac equation with a δ function interaction. The time dependent solution is then given in terms of Lommel functions of two variables [10,11] and its Fourier transform will allow comparison with the perturbative approach for relativistic particles [12].

Appendix

The diffraction in time wave functions

In an old paper [4], one of the authors (M.M.) discussed, from the standpoint of quantum mechanics, the transient effects in a particle current when one opens a shutter.

The mathematical problem concerned the determination of a wave function $\chi(x,k,t)$ that satisfies the free particle, one dimensional, time dependent Schrödinger equation

$$i\frac{\partial\chi}{\partial t} = -\frac{1}{2}\frac{\partial^2\chi}{\partial x^2}, \tag{A.1}$$

with the initial value

$$\chi(x,k,0) = \begin{cases} 2\exp(ikx) & \text{if } x < 0 \\ 0 & \text{if } x > 0. \end{cases} \tag{A.2}$$

This problem can be solved using the Laplace transform

$$\bar{\chi}(x,k,s) = \int_0^\infty e^{-st}\chi(x,k,t)dt, \tag{A.3}$$

which, by a reasoning similar to the one leading to Eq. (3.3) of the present paper, satisfies the equations

$$\left(-\frac{1}{2}\frac{d^2}{dx^2} - is\right)\bar{\chi}(x,k,s) = \begin{cases} -2ie^{ikx} & \text{if } x < 0 \\ 0 & \text{if } x > 0. \end{cases} \tag{A.4}$$

As in (3.4), a solution to these equations can be written in the form

$$\bar{\chi}(x,k,s) = \begin{cases} A_-e^{-i(2is)^{1/2}x} + Be^{ikx} & \text{if } x < 0 \\ A_+e^{i(2is)^{1/2}x} & \text{if } x > 0. \end{cases} \tag{A.5}$$

From equation (A.4), when $x < 0$, we have that

$$B = -2i\left(\frac{1}{2}k^2 - is\right)^{-1}, \tag{A.6}$$

while requiring the continuity of the solution and its derivative at $x = 0$ gives us

$$A_+ = \frac{2i}{(2is)^{1/2}[(2is)^{1/2} - k]}, \qquad A_- = \frac{-2i}{(2is)^{1/2}[(2is)^{1/2} + k]}. \tag{A.7}$$

Thus using the inverse Laplace transform we obtain for $x > 0$ that

$$\chi(x,k,t) = \frac{1}{2\pi i}\int_{c-i\infty}^{c+i\infty} \frac{(2i)e^{i(2is)^{1/2}x}e^{st}ds}{(2is)^{1/2}[(2is)^{1/2} - k]}. \tag{A.8}$$

Replacing the positive x by its absolute value $|x|$, we obtain the relation (3.14) of the paper, and while the explicit expression $\chi(x,k,t)$ given in Ref. [4] was discussed for k real and positive, the relation (A.8) is valid for any complex k so long as c is larger than the real part of $-ik^2/2$. The functional form [4] of $\chi(|x|,k,t)$ is reproduced in Eq. (3.15) of this paper.

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Resumen. Cuando de discute la teoría de perturbaciones dependiente del tiempo, los estudiantes ocasionalmente preguntan si hay ecuaciones de Schrödinger dependientes del tiempo que puedan resolverse exactamente. Sugieren que de ser eso posible permitiría la comparación entre las transiciones perturbativas y las exactas inducidas por una interacción. En este trabajo implementamos el programa anterior para un hamiltoniano en un espacio unidimensional que contiene a la energía cinética más un potencial delta de interacción. Las soluciones exactas se obtienen con ayuda de las encontradas hace muchos años para el problema de difracción en el tiempo y, como era de esperarse, coinciden con el resultado perturbativo para tiempos largos e interacciones débiles. En la sección final indicamos que la validez de nuestras conclusiones es más general que el sencillo ejemplo con que se ilustran en este trabajo.