

Solution of the Schrödinger Equation for a Linear Potential using the Extended Baker-Campbell-Hausdorff Formula

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Abstract: The time-dependent Schrödinger equation is solved for a linear potential using operational methods; in particular, an extension of the Baker-Campbell-Hausdorff formula is exposed and used. Several initial conditions are considered. A closed form for the Wigner function is presented. The results can be extended to the propagation of an electromagnetic field in the paraxial approximation.

Keywords: Schrödinger equation, linear potential, Zassenhaus formula, Baker-Campbell-Hausdorff formula, Wigner function

1 Introduction

The main problem of non-relativistic quantum mechanics is the solution of the Schrödinger equation; several exact analytical, approximated analytic and numerical methods have been invented for this purpose [1,2,3]. Between the exact analytical methods, we can count the ones based on operator techniques; such methods are relatively new and can give very simple solutions, to otherwise complicated approaches [4,5,6,7]. That is the case of the linear potential; the solution of the Schrödinger equation for the linear potential is very well known, but it has been neglected in the quantum mechanics books [8,9]. The time dependent solution is usually done in terms of the eigenfunctions of the Hamiltonian, the Airy functions, as an integral over the continuous eigenvalue, the energy; however, an explicit solution for a given initial condition is not normally presented.

In this work, we use operator techniques to find an exact analytic solution of the time-dependent Schrödinger equation with a linear potential $V(x) = Fx$. We solve the problem for several initial conditions. To do that, we use a very easy and direct generalization of the Baker-Campbell-Hausdorff formula [4,7,10], that is derived from the Zassenhaus formula [11,12,10]. This extended Baker-Campbell-Hausdorff formula allows us to disentangle the evolution operator, and to analyze the

action of this operator over initial conditions adequately written.

The explicit solution that it is found, allows us to write a closed form for the Wigner function in terms of the Fourier transform of the initial condition. The Wigner function can then be calculated for the initial conditions that we present; as the results are very cumbersome, we present only the case when the initial condition is an Airy function.

The Schrödinger equation for the linear potential mimics exactly the paraxial equation in two dimensions [13,14,15]; so, our results works perfectly well for beam propagation under the influence of a linear gradient refractive index [16].

2 The formal solution of the Schrödinger equation for a linear potential using operators

The one dimensional Schrödinger equation for a linear potential $V(x) = Fx$ is

$$i \frac{\partial \psi(x,t)}{\partial t} = \left(\frac{\hat{p}^2}{2} + F\hat{x} \right) \psi(x,t), \quad (1)$$

where \hat{x} and \hat{p} are two Hermitian operators (i.e., two non-commuting variables) with the commutation relation

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$[\hat{x}, \hat{p}] = i$ [1,2,3]. We will use a unit system where $\hbar = 1$ and the mass $m = 1$.

As the Hamiltonian is time independent, equation (1) can be integrated with respect to time, and the formal solution found as

$$\psi(x,t) = \exp \left\{ -it \left(\frac{\hat{p}^2}{2} + Fx \right) \right\} \psi(x,0), \quad (2)$$

where $\psi(x,0)$ is the initial condition, namely, the state of the system at time $t = 0$.

3 The extended Baker-Campbell-Hausdorff formula

The Zassenhaus formula establishes [11, 12, 10] that

$$e^{\lambda(\hat{X}+\hat{Y})} = e^{\lambda\hat{X}} e^{\lambda\hat{Y}} e^{\lambda^2 C_2(\hat{X},\hat{Y})} e^{\lambda^3 C_3(\hat{X},\hat{Y})} e^{\lambda^4 C_4(\hat{X},\hat{Y})} \dots, \quad (3)$$

where \hat{X} and \hat{Y} are two operators, that is, two non-commuting variables, and

$$C_2(\hat{X},\hat{Y}) = -\frac{1}{2} [\hat{X}, \hat{Y}], \quad (4)$$

$$C_3(\hat{X},\hat{Y}) = \frac{1}{3} [\hat{Y}, [\hat{X}, \hat{Y}]] + \frac{1}{6} [\hat{X}, [\hat{X}, \hat{Y}]], \quad (5)$$

$$C_4(\hat{X},\hat{Y}) = -\frac{1}{8} ([\hat{Y}, [\hat{Y}, [\hat{X}, \hat{Y}]]] + [\hat{Y}, [\hat{X}, [\hat{X}, \hat{Y}]]]) - \frac{1}{24} [\hat{X}, [\hat{X}, [\hat{X}, \hat{Y}]]], \quad (6)$$

and so on. The general expression for $C_i(\hat{X},\hat{Y})$ is very complicated and we don't need it here (See [11] and references there in).

If $[\hat{Y}, [\hat{X}, \hat{Y}]] = 0$ and $[\hat{X}, [\hat{X}, \hat{Y}]] = 0$, $C_3[\hat{X}, \hat{Y}] = 0$, all the subsequent C 's are also zero, and we got the well known Baker-Campbell-Hausdorff formula

$$e^{\lambda(\hat{X}+\hat{Y})} = e^{\lambda\hat{X}} e^{\lambda\hat{Y}} e^{-\frac{\lambda^2}{2} [\hat{X}, \hat{Y}]} \quad (7)$$

If at least one of the two $[\hat{Y}, [\hat{X}, \hat{Y}]]$ or $[\hat{X}, [\hat{X}, \hat{Y}]]$ are different from zero, and $[\hat{Y}, [\hat{Y}, [\hat{X}, \hat{Y}]]] = 0$, $[\hat{Y}, [\hat{X}, [\hat{X}, \hat{Y}]]] = 0$, $[\hat{X}, [\hat{X}, [\hat{X}, \hat{Y}]]] = 0$, only C_2 and C_3 will be different from zero, and all the others subsequent C 's will be zero, obtaining the extended Baker-Campbell-Hausdorff formula

$$e^{\lambda(\hat{X}+\hat{Y})} = e^{\lambda\hat{X}} e^{\lambda\hat{Y}} e^{-\frac{\lambda^2}{2} [\hat{X}, \hat{Y}]} e^{\frac{\lambda^3}{3!} (2[\hat{Y}, [\hat{X}, \hat{Y}]] + [\hat{X}, [\hat{X}, \hat{Y}]])}. \quad (8)$$

There is also a "left oriented" version of the Zassenhaus formula that is as useful as the normal one, that gives us left oriented versions of the Baker-Campbell-Hausdorff formula and of the extended Baker-Campbell-Hausdorff

formula. The "left oriented" version of the Baker-Campbell-Hausdorff formula is

$$e^{\lambda(\hat{X}+\hat{Y})} = e^{\frac{\lambda^2}{2} [\hat{X}, \hat{Y}]} e^{\lambda\hat{Y}} e^{\lambda\hat{X}} \quad (9)$$

and the "left oriented" extended Baker-Campbell-Hausdorff formula is

$$e^{\lambda(\hat{X}+\hat{Y})} = e^{\frac{\lambda^3}{3!} (2[\hat{Y}, [\hat{X}, \hat{Y}]] + [\hat{X}, [\hat{X}, \hat{Y}]])} e^{\frac{\lambda^2}{2!} [\hat{X}, \hat{Y}]} e^{\lambda\hat{Y}} e^{\lambda\hat{X}}. \quad (10)$$

4 Application of the extended Baker-Campbell-Hausdorff formula to the Schrödinger equation with a linear potential

We apply now expression (10) to the formal solution (2). For that, we choose $\lambda = -it$, $\hat{X} = \frac{\hat{p}^2}{2}$, and $\hat{Y} = Fx$; we have

$$[\hat{X}, \hat{Y}] = i\frac{F}{2}\hat{p}, \quad (11)$$

$$[\hat{X}, [\hat{X}, \hat{Y}]] = 0, \quad [\hat{Y}, [\hat{X}, \hat{Y}]] = F^2, \quad (12)$$

and

$$[\hat{Y}, [\hat{Y}, [\hat{X}, \hat{Y}]]] = 0, \quad (13)$$

$$[\hat{Y}, [\hat{X}, [\hat{X}, \hat{Y}]]] = 0 \quad (14)$$

$$[\hat{X}, [\hat{X}, [\hat{X}, \hat{Y}]]] = 0 \quad (15)$$

so actually, we can apply the left oriented extended Baker-Campbell-Hausdorff formula (10). Using (11) and (12), we find $C_2' = -i\frac{F}{2}\hat{p}$ and $C_3' = \frac{F^2}{3}$, so

$$\psi(x,t) = \exp\left(i\frac{F^2 t^3}{3}\right) \exp\left(i\frac{F t^2}{2}\hat{p}\right) \exp(-iFtx) \exp\left(-i\frac{t}{2}\hat{p}^2\right) \psi(x,0). \quad (16)$$

Using the Hadamard lemma [4,7,10], it is easy to show that $\exp\left(-i\frac{t}{2}\hat{p}^2\right) \psi(x,0) = \psi(x-t\hat{p},0)$ and that for an arbitrary well behaved function f , we have $\exp\left(i\frac{F t^2}{2}\hat{p}\right) f(x) = f\left(x + \frac{F t^2}{2}\right)$; thus,

$$\psi(x,t) = \exp\left[-i\frac{Ft(Ft^2+6x)}{6}\right] \psi\left(x + \frac{Ft^2}{2} - t\hat{p}, 0\right) 1. \quad (17)$$

5 Writing the initial condition as a Fourier transform

Now, we write the initial condition in terms of its Fourier transform; i.e., we write

$$\psi(x,0) = \int_{-\infty}^{\infty} dv Y(v) \exp(-2\pi i xv), \quad (18)$$

and we substitute it in equation (17), obtaining

$$\psi(x,t) = \int_{-\infty}^{\infty} dv Y(v) \exp(-i\pi v F t^2) \exp[2\pi i v (x - t\hat{p})] 1; \tag{19}$$

the operator in the last exponential can be disentangled using the Baker-Campbell-Hausdorff formula [4, 7, 10], and after some trivial algebra one gets

$$\psi(x,t) = \exp\left[-i\frac{Ft(Ft^2 + 6x)}{6}\right] \int_{-\infty}^{\infty} dv Y(v) e^{-i\pi v F t^2} \exp\left\{2\pi i \left[\left(x + \frac{Ft^2}{2}\right)v - \pi t v^2\right]\right\}, \tag{20}$$

where

$$Y(v) = \int_{-\infty}^{\infty} d\xi \psi(\xi, 0) \exp(-2\pi i \xi v). \tag{21}$$

6 Some particular initial conditions

6.1 Initial condition: $\psi(x, 0) = A \exp(ikx)$

We treat now the case when the initial state of the system is a plane wave, namely $\psi(x, t = 0) = e^{ikx}$. It is a very easy exercise in this case to find that

$$\psi(x,t) = A \exp\left[i\left(kx + \frac{Fkt^2}{2} - \frac{F^2t^3}{6} - Ftx - \frac{k^2t}{2}\right)\right]. \tag{22}$$

This solution satisfies the Schrödinger equation (1) and the initial condition $\psi(x, t = 0) = e^{ikx}$, so it is the solution.

6.2 Initial condition: $\psi(x, 0) = Ae^{-a(x-b)^2}$

When the initial condition is a Gaussian function $\psi(x, 0) = A \exp[-a(x - b)^2]$, the Fourier transform is also a Gaussian, and substituting it in expression (20), we obtain after easy, but cumbersome, calculations

$$\psi(x,t) = \frac{A}{\sqrt{1 + 2iat}} \exp[g_1(t) + g_2(t) + g_3(t)], \tag{23}$$

where

$$g_1(t) = -\frac{i(-12ab^2 + 12abFt^2 + aF^2t^4 - 2iF^2t^3)}{12(2at - i)}, \tag{24}$$

$$g_2(t) = -\frac{ix(2ab + aFt^2 - iFt)}{2at - i}, \tag{25}$$

and

$$g_3(t) = \frac{ax^2}{-1 - 2iat}. \tag{26}$$

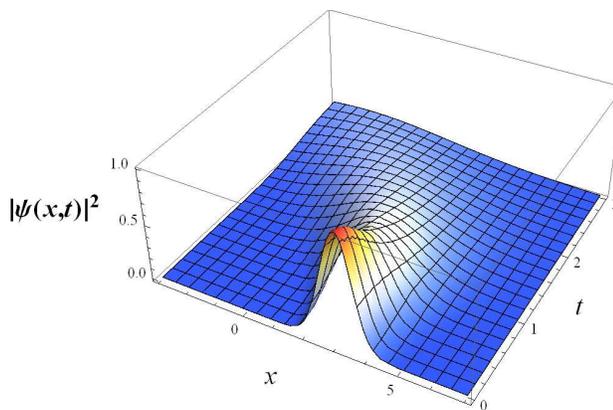


Fig. 1: The solution $|\psi(x,t)|^2$, when the initial condition is $\psi(x,0) = Ae^{-a(x-b)^2}$, with $F = 1, A = 1, a = 1$, and $b = 3$.

Again it is not difficult to show that the initial condition is fulfilled and that equation (1) is satisfied. In Figure 1, we show the squared amplitude as a function of the position x and as a function of time t , when $F = 1, A = 1, a = 1$, and $b = 3$. We observe that the peak of $|\psi(x,t)|^2$ goes to lower values of x ; if the sign of F is inverted, the motion of the peak is reversed, going in that case to the greater values of x , as expected.

6.3 Initial condition: $\psi(x, 0) = Ai(ax)$

In this case, we get $F(v) = \frac{1}{a} \exp\left(i\frac{8\pi^3 v^3}{3a^3}\right)$, that inserted in (20) take us to

$$\psi(x,t) = \frac{1}{2\pi a} \exp\left[-i\left(\frac{F^2t^3}{6} + Ftx\right)\right] \int_{-\infty}^{\infty} dv \exp\left[i\left(\frac{v^3}{3a^3} + xv + \frac{Ft^2}{2}v - \frac{t}{2}v^2\right)\right], \tag{27}$$

that after some trivial algebra can be cast as

$$\psi(x,t) = \frac{1}{2\pi a} \exp\left[-i\left(\frac{F^2t^3}{6} + Ftx - \frac{a^6t^3}{24}\right)\right] \int_{-\infty}^{\infty} dv \exp\left[\frac{i}{3a^3}\left(v - \frac{a^3t}{2}\right)^3 + \left(x - \frac{a^3t^2}{4} + \frac{Ft^2}{2}\right)v\right]. \tag{28}$$

Using the integral representation [17, 18]

$$Ai(x) = \frac{1}{2\pi} \int_{-\infty}^{\infty} \exp\left[i\left(\frac{u^3}{3} + xu\right)\right] du, \tag{29}$$

that it is valid for x real, we finally arrive to

$$\psi(x,t) = \exp \left\{ -i \frac{t}{12} (a^3 - 2F) [t^2 (a^3 - F) - 6x] \right\} \text{Ai} \left[ax - \frac{1}{4} at^2 (a^3 - 2F) \right] \tag{30}$$

Figure 2 displays $|\psi(x,t)|^2$ when $F = 1$, and $a = 1$. As in

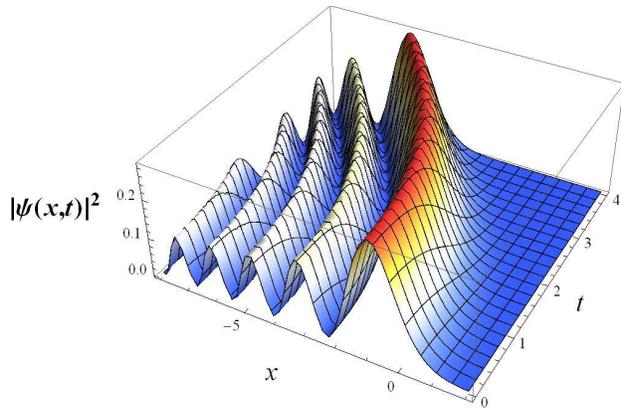


Fig. 2: The solution $|\psi(x,t)|^2$, when the initial condition is $\psi(x,0)=\text{Ai}(ax)$, with $F = 1$ and $a = 1$.

the previous case, the direction of the twist of the maximum of the probability distribution is inverted when we change the sign of F .

6.4 Initial condition: $\psi(x,0) = e^{-cx^2} \text{Ai}(ax)$

First, the Fourier transform is calculated using the convolution theorem; second, it is substituted in (20); third, the integral representation (29) of the Airy function is used, and finally

$$\psi(x,t) = \frac{1}{\sqrt{1+2ict}} \exp[h_1(t) + h_2(t) + h_3(t)] \text{Ai}[h_4(t)] \tag{31}$$

where

$$h_1(t) = \frac{t^3}{12(2ct-i)^3} [a^6 - 3a^3F(1+2ict) + 2F^2] - \frac{icF^2t^4(-2ct+3i)^2}{12(2ct-i)^3} \tag{32}$$

$$h_2(t) = -\frac{itx(a^3 + 4c^2Ft^2 - 6icFt - 2F)}{2(2ct-i)^2}, \tag{33}$$

$$h_3(t) = \frac{cx^2}{-1-2ict}, \tag{34}$$

and

$$h_4(t) = \frac{a[a^3t^2 - 2i(2ct-i)(Ft^2 + 2x)]}{4(-2ct+i)^2}. \tag{35}$$

The behavior of the solution in this case is presented in

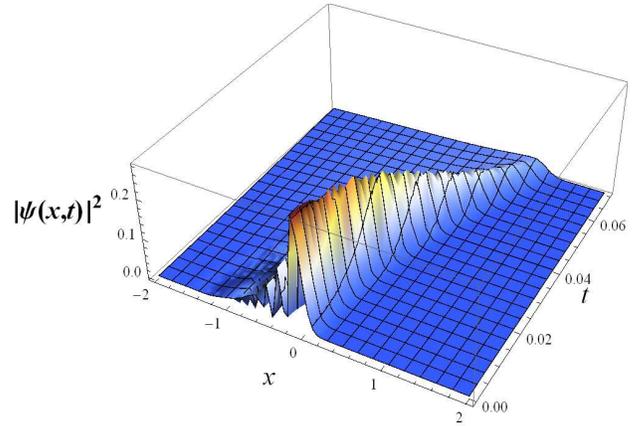


Fig. 3: The solution $|\psi(x,t)|^2$, when the initial condition is $\psi(x,0)=e^{-cx^2} \text{Ai}(ax)$, with $F = 1$, $c = 1$, and $a = 1$.

Figure 3 for $F = 1$, $c = 1$, and $a = 1$. The same observation made in the previous cases about the behavior of $|\psi(x,t)|^2$ with respect to the sign of F is valid.

7 Initial condition: $\psi(x,0) = J_n(ax)$

When the initial condition is a Bessel function of the first kind, we can not use directly equation (20) because we do not know the Fourier transform, so we go back to expression (16) and we write [18, 19]

$$J_n(ax) = \frac{1}{2\pi} \int_{-\pi}^{\pi} \exp(in\tau) \exp[-iax \sin(\tau)] d\tau, \tag{36}$$

to obtain

$$\psi(x,t) = \exp\left(i \frac{F^2 t^3}{3}\right) \exp\left(i \frac{F t^2}{2} \hat{p}\right) \exp(-iFtx) \exp\left(-i \frac{t}{2} \hat{p}^2\right) \frac{1}{2\pi} \int_{-\pi}^{\pi} e^{in\tau} \exp[-iax \sin(\tau)] d\tau. \tag{37}$$

Following the same procedure that took us from equation (16) to equation (17), we arrive to

$$\psi(x,t) = \frac{1}{2\pi} \exp\left[i\left(-\frac{F^2 t^3}{6} - Ftx\right)\right] \int_{-\pi}^{\pi} \exp\left\{i\left[n\tau - \frac{aFt^2 \sin(\tau)}{2} - xa \sin(\tau) - \frac{ta^2 \sin^2(\tau)}{2}\right]\right\} d\tau \tag{38}$$

From here, we make

$$\sin^2 \tau = \frac{1}{2}[1 - \cos(2\tau)] = \frac{1}{4}[2 - e^{2i\tau} - e^{-2i\tau}],$$

to get

$$\begin{aligned} \psi(x,t) &= \frac{1}{2\pi} \exp\left[i\left(-\frac{F^2 t^3}{6} - Ftx\right)\right] \\ &\int_{-\pi}^{\pi} \exp\left(-\frac{ia^2 t}{4}\right) \exp\left\{i\left[n\tau - \left(\frac{Ft^2}{2} + x\right)a \sin(\tau)\right]\right\} \\ &\exp\left[i\left(\frac{a^2 t}{8} e^{2i\tau}\right)\right] \exp\left[i\left(\frac{a^2 t}{8} e^{-2i\tau}\right)\right] d\tau, \end{aligned} \quad (39)$$

we write the last two exponentials inside the integral in terms of their Taylor series,

$$\begin{aligned} \psi(x,t) &= \exp\left[i\left(-\frac{F^2 t^3}{6} - Ftx - \frac{a^2 t^2}{4}\right)\right] \\ &\sum_{j,k=0}^{\infty} \frac{1}{j!k!} \left(\frac{ia^2 t}{8}\right)^{j+k} \\ &\frac{1}{2\pi} \int_{-\pi}^{\pi} \exp\left\{i\left[(n+2j-2k)\tau - \left(\frac{Ft^2}{2} + x\right)a \sin(\tau)\right]\right\} d\tau. \end{aligned} \quad (40)$$

Recalling (36), we obtain

$$\begin{aligned} \psi(x,t) &= \exp\left[i\left(-\frac{F^2 t^3}{6} - Ftx - \frac{a^2 t^2}{4}\right)\right] \\ &\sum_{j,k=0}^{\infty} \frac{1}{j!k!} \left(\frac{ia^2 t}{8}\right)^{j+k} J_{n+2j-2k} \left[a\left(x + \frac{Ft^2}{2}\right)\right]. \end{aligned} \quad (41)$$

Changing the index in the j sum to $M = j - k$,

$$\begin{aligned} \psi(x,t) &= \exp\left[i\left(-\frac{F^2 t^3}{6} - Ftx - \frac{a^2 t^2}{4}\right)\right] \\ &\sum_{k=0}^{\infty} \sum_{M=-k}^{\infty} \frac{1}{(M+k)!k!} \left(\frac{ia^2 t}{8}\right)^{M+2k} \\ &J_{n+2(M+k)-2k} \left[a\left(x + \frac{Ft^2}{2}\right)\right]; \end{aligned} \quad (42)$$

the M sum can be extended from $-\infty$, since we are adding zeros to the sum ($\frac{1}{\eta!} = 0$, when η is a negative integer), and using that

$$J_M\left(\frac{a^2 t}{4}\right) = \sum_{k=0}^{\infty} \frac{(-1)^k}{(M+k)!k!} \left(\frac{ia^2 t}{8}\right)^{M+2k}, \quad (43)$$

we obtain the final result

$$\begin{aligned} \psi(x,t) &= \exp\left[-i\left(Ftx + \frac{F^2 t^3}{6} + \frac{a^2 t^2}{4}\right)\right] \\ &\sum_{M=-\infty}^{\infty} i^M J_{n+2M} \left[a\left(x + \frac{Ft^2}{2}\right)\right] J_M\left(\frac{a^2 t}{4}\right). \end{aligned} \quad (44)$$

The initial condition $\psi(x,0) = J_n(ax)$ is realized, and with some work, it can be verified that (1) is fulfilled. Figures 4, 5 and 6 show $|\psi(x,t)|^2$ when $F = 1$, and $a = 1$ for $n = 0$, $n = 1$, and $n = 7$, respectively.

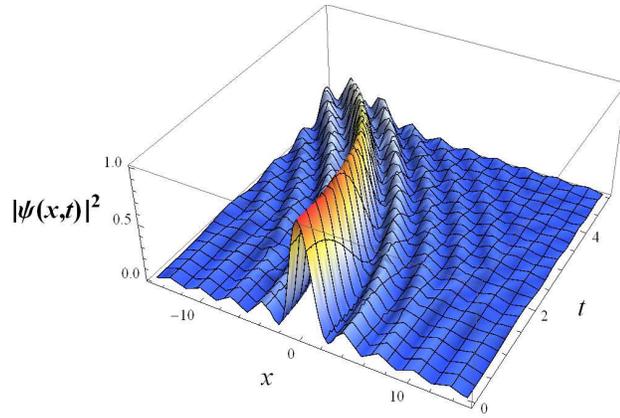


Fig. 4: The solution $|\psi(x,t)|^2$, when the initial condition is $\psi(x,0)=J_n(ax)$, with $F = 1$, $n = 0$, and $a = 1$.

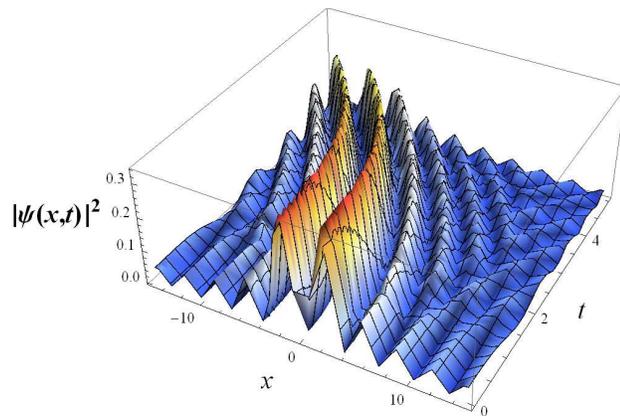


Fig. 5: The solution $|\psi(x,t)|^2$, when the initial condition is $\psi(x,0)=J_n(ax)$, with $F = 1$, $n = 1$, and $a = 1$.

8 The Wigner function

Being the Wigner function [20] one of the most know quasiprobability distribution functions [21,22], we want to study it next. Using formula (20), the Wigner function [20]

$$W(x,p) = \frac{1}{\pi} \int_{-\infty}^{\infty} dy \psi^*(x+y) \psi(x-y) \exp(2ipy) \quad (45)$$

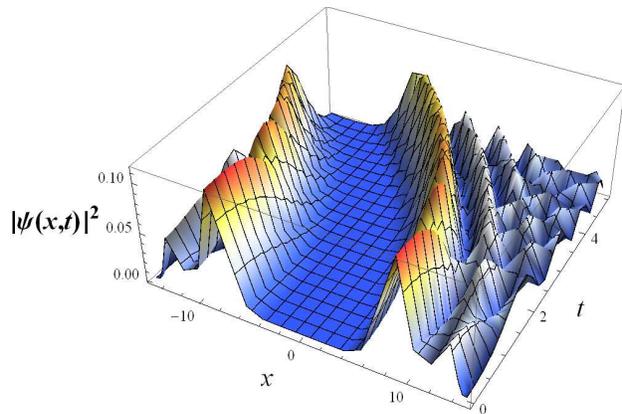


Fig. 6: The solution $|\psi(x,t)|^2$, when the initial condition is $\psi(x,0)=J_n(ax)$, with $F = 1$, $n = 7$, and $a = 1$.

can be calculated in terms of the Fourier transform of any reasonable initial condition as

$$W(x,p) = \frac{1}{\pi} \exp \left\{ \frac{i}{\pi} (Ft+p) \left[Ft^3 (Ft+p)^2 + 2\pi x \right] \right\} \int_{-\infty}^{\infty} dv Y^*(v) Y \left(\frac{p}{\pi} + \frac{Ft}{\pi} - v \right) \exp \left(-4iv \left\{ Ft^3 (Ft+p)^2 - \pi [Ft^3 v (Ft+p) - x] \right\} \right), \quad (46)$$

where $Y(v)$ has the same meaning of the previous sections.

We present explicitly the case when the initial condition is an Airy function, $\psi(x,0) = \text{Ai}(ax)$; in this case,

$$W(x,p) = \frac{1}{2^{1/3}} \text{Ai} \left[\frac{2(Ft+p)^2 - a^3 (Ft^2 + 2pt - 2x)}{\sqrt[3]{2}a^2} \right] \quad (47)$$

In Figure 7, we show the Wigner function at different

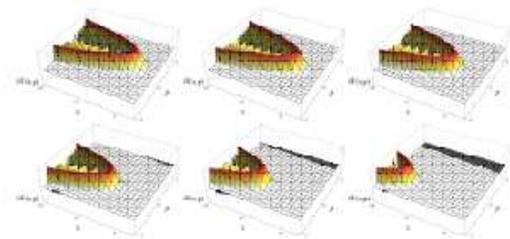


Fig. 7: The Wigner function for the Airy function as initial condition with $F = 1$ and $a = 1$, for t from 0 to 5 in 1 steps.

times (t from 0 to 5 in 1 steps) when $F = 1$ and $a = 1$.

Since the Wigner function is only non-negative for Gaussian states [23,24], it presents large regions where it is negative, as expected. With time the Wigner function moves but it keeps its initial form (Figure 8).

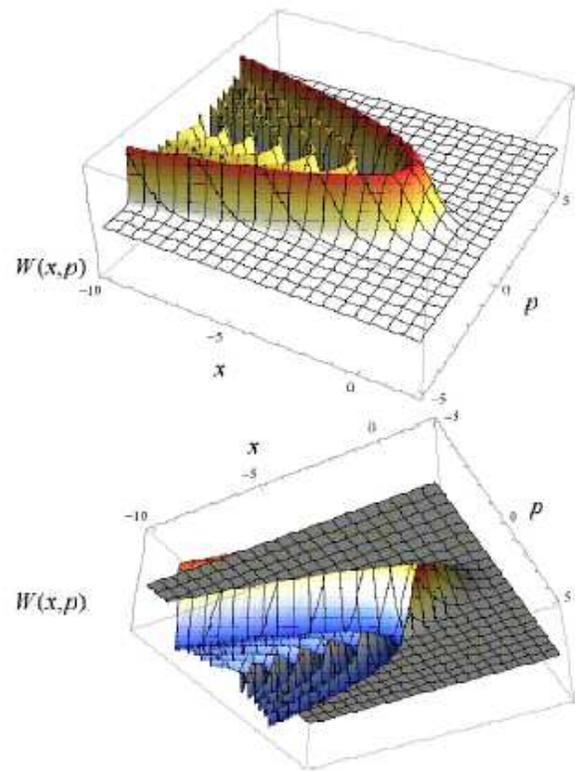


Fig. 8: The Wigner function when the initial condition is an Airy function with $a = 1$ and when $F = 1$ for $t = 1$.

9 Conclusions

The operational methods are very easy to understand, and in some conditions, also very easy to apply. In this work, we present a direct generalization of the Baker-Campbell-Hausdorff formula from the Zassenhaus formula and we use it to solve the time-dependent Schrödinger equation for a linear potential for arbitrary initial condition, without solving the corresponding stationary Schrödinger equation. The Wigner function can be found and all physically measurable quantities can be calculated directly from it.

As the paraxial equation for a linear GRIN medium is also (1), with the adequate substitutions (axial coordinate z substitutes time t), these results can also be useful in optics, in particular, the Wigner function.

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