The particle in the box: Intermode traces in the propagator

I. Marzoli, I. Bialynicki-Birula∗, O. M. Friesch, A. E. Kaplan† and W. P. Schleich
Abteilung für Quantenphysik, Universität Ulm, 89069 Ulm, Germany

Characteristic structures such as canals and ridges—inter mode traces—emerge in the spacetime representation of the probability distribution of a particle in a one-dimensional box. We show that the corresponding propagator already contains these structures. We relate their visibility to the factorization property of the initial wave packet.

I. INTRODUCTION

The Zeeman or Stark effect in a hydrogen atom [1], the phase change at a conical intersection in a polyatomic molecule [2] and the nuclear shell structure [3] are three striking phenomena illustrating the importance of degeneracies in quantum mechanics. But how can degeneracies play a key role in such a well-studied problem as the particle in the box? In the present paper we show that the characteristic structures [4–9] in the spacetime representation of a particle in a box shown in Figs. 1 and 2 and referred to as quantum carpet are a consequence of a manifold degeneracy [10].

Our analysis relies on three observations:

(i) The wave function of the particle at time \( t \) is the integral of the initial wave function and the well known propagator of the box problem [1].

(ii) The probability of finding the particle is the absolute value squared of the wave function. In the propagator formulation of quantum mechanics this translates into the two-dimensional integral of the product of the initial wave function and its complex conjugate multiplied by a kernel. This kernel is the product of the Green’s function and its complex conjugate evaluated at the two different initial conditions.

(iii) The quadratic dependence of the energy on the quantum number factorizes in the product of the Green’s functions into the product of two linear dependences.

These observations allow us to rewrite the kernel in a way which brings out most clearly that the carpet structure is inherent to the propagator. Three results stand out:

(i) The kernel is only non-vanishing along straight lines in spacetime.

(ii) The steepness of these lines is discrete.

(iii) These lines either start at the difference or the sum of the integration variables.

But where is the degeneracy? The first degeneracy has its roots in the dispersion relation connecting in a quadratic way kinetic energy and wave number. This forces many quantum numbers to contribute to the same spacetime line. Another degeneracy arises when the product of the initial wave function times its complex conjugate factorizes into the product of two functions which now contain the sum and the difference of the integration variables, only. This degeneracy in the initial wave function either enhances or suppresses the intermode traces resulting from the spectrum degeneracy. We note that the phenomenon of fractional revivals [5,11,12] is closely related to the intermode traces.

Our paper is organized as follows. In Sec. II we cast the probability to find the particle at time \( t \) at the position \( x \) in the box into a kernel formulation. Within Sec. III we rewrite this kernel to bring out the intermode traces and discuss in Sec. IV the consequences of the factorization property for the emergence of the carpet. We illustrate these results in Sec. V for the example of a Gaussian wave packet. We conclude in Sec. VI by summarizing our main results and giving an outlook.

∗Permanent address: Center for Theoretical Physics, Lotników 46, 02–668 Warsaw, Poland
†Permanent address: Electr. & Comp. Eng. Dept., The Johns Hopkins University, MD–21210, USA
II. THE PARTICLE IN THE BOX: A BRIEF SUMMARY

In this section we briefly summarize the essential ingredients of the problem of the particle in the box. In particular, we express the probability $W(x,t)$ to find the particle at time $t$ at position $x$ as an integral of the product of the initial wave packet, its complex conjugate and a kernel. This kernel is the product of the two Green’s functions at two different initial positions.

We consider the motion of a particle of mass $M$ caught between two walls separated by a length $L$. The wave function $\psi(x,t)$ of this particle at time $t$ reads

$$\psi(x,t) = \sum_{m=1}^{\infty} \psi_m u_m(x) \exp(-i E_m t/\hbar).$$

(1)

Here the expansion coefficients

$$\psi_m \equiv \int_0^L dx' u_m(x') \varphi(x')$$

(2)

follow from the wave function $\psi(x,t=0) \equiv \varphi(x)$ at time $t=0$ and from the energy eigenfunctions

$$u_m(x) \equiv \mathcal{N} \sin(k_m x) \equiv \sqrt{2/L} \sin\left(\frac{m \pi x}{L}\right)$$

(3)

with eigenvalue

$$E_m \equiv \frac{(hk_m)^2}{2M} = m^2 \hbar \frac{2\pi}{T}.$$  

(4)

Here we have introduced the revival time $T \equiv 4ML^2/(\pi \hbar)$.

Note that the form of the energy eigenfunctions $u_m$ together with the wave numbers $k_m$ guarantee that the wave function $\psi$ satisfies the boundary conditions

$$\psi(x=0,t) = \psi(x=L,t) = 0$$

(5)

enforced by the two walls at $x=0$ and $x=L$ at all times.

The constant $\mathcal{N} \equiv (2/L)^{1/2}$ results from the normalization condition

$$1 = \int_0^L dx u_m(x)^2 = \mathcal{N}^2 \int_0^L dx \frac{1}{2} [1 - \cos(2k_m x)] = \mathcal{N}^2 \frac{L}{2}.$$  

(6)

For further calculations it is more convenient to have the summation in the representation Eq. (1) of the wave function run from minus infinity to plus infinity rather than from unity to plus infinity. For this purpose we first decompose the energy eigenfunctions

$$u_m(x) = \sqrt{\frac{1}{2L}} \left( e^{im\pi x/L} - e^{-im\pi x/L} \right)$$

(7)

into right and left running waves which yields

$$\psi(x,t) = \frac{1}{i\sqrt{2L}} \sum_{m=1}^{\infty} \left\{ \psi_m \exp\left[ i\pi m \left( \frac{x}{L} - m \frac{2t}{T} \right) \right] - \psi_m \exp\left[ -i\pi m \left( \frac{x}{L} + m \frac{2t}{T} \right) \right] \right\}.$$  

(8)

When we define the expansion coefficients $\psi_m$ for negative values of $m$ by

$$\psi_{-|m|} \equiv -\psi_{|m|}$$

(9)

we find the compact representation

$$\psi(x,t) = \frac{1}{i\sqrt{2L}} \sum_{m=-\infty}^{\infty} \psi_m \exp\left[ i\pi m \left( \frac{x}{L} - m \frac{2t}{T} \right) \right]$$

(10)
of the wave function. Here we have used the fact that \( \psi_0 = 0 \) since \( u_0 = 0 \).

When we now substitute the explicit form

\[
\psi_m = \frac{1}{i\sqrt{2L}} \int_0^L dx' \left[ \exp\left(i\pi m \frac{x'}{L}\right) - \exp\left(-i\pi m \frac{x'}{L}\right) \right] \varphi(x')
\]

of the expansion coefficients into the expression Eq. (10) of the wave function we arrive at

\[
\psi(x, t) = \int_0^L dx' \varphi(x') G(x, t | x').
\]

Here we have introduced the Green’s function

\[
G(x, t | x') \equiv \frac{1}{2L} \sum_{m=-\infty}^{\infty} \left[ \exp\left(-i\pi m \frac{x'}{L}\right) - \exp\left(i\pi m \frac{x'}{L}\right) \right] \times \exp\left[i\pi m \left(\frac{x}{L} - \frac{m^2 t}{T}\right)\right]
\]

of the particle in the box.

With the help of this result we can represent the probability

\[
W(x, t) = |\psi(x, t)|^2 = \int_0^L dx' \int_0^L dx'' \varphi^*(x') \varphi(x'') K(x, t | x', x'')
\]

to find the particle at time \( t \) at the position \( x \) in terms of the initial wave function \( \varphi \), its complex conjugate \( \varphi^* \) and the kernel

\[
K(x, t | x', x'') \equiv G^*(x, t | x') \cdot G(x, t | x'')
\]

consisting of the product of the two Green’s functions at the two different initial positions.

In the next section we show that the kernel already contains the intermode traces in the carpet. They emerge in a striking way provided the initial wave packet satisfies an appropriate factorization condition.

### III. A NEW REPRESENTATION OF THE KERNEL

In this section we first find a new representation of the kernel. We then discuss its properties. For the details of the calculations we refer to the appendix.

We first calculate the kernel defined in Eq. (15). For this purpose we substitute the expression Eq. (13) for the Green’s function \( G \) and an analogous expression for \( G^* \) into the definition, Eq. (15), of the kernel. After minor algebra we arrive at

\[
K(x, t | x', x'') = \frac{1}{4L^2} \sum_{m', m''=-\infty}^{\infty} \exp\left\{-i\pi (m' - m'') \left(\frac{x}{L} - (m' + m'') \frac{2t}{T}\right)\right\} \\
\times \left\{ \exp\left[i\pi \left(\frac{m' x'}{L} - m'' x''\right)\right] + \exp\left[-i\pi \left(\frac{m' x'}{L} - m'' x''\right)\right] \right. \\
- \exp\left[i\pi \left(\frac{m x'}{L} + m'' x''\right)\right] - \exp\left[-i\pi \left(\frac{m x'}{L} + m'' x''\right)\right] \right\}.
\]

When we recall the relations

\[
m' x' - m'' x'' = (m' - m'') \frac{x' + x''}{2} + (m' + m'') \frac{x' - x''}{2}
\]

and

\[
m' x' + m'' x'' = (m' + m'') \frac{x' + x''}{2} + (m' - m'') \frac{x' - x''}{2}
\]

we can cast the kernel into the form
\[ K(x, t \mid x', x'') = \frac{1}{4L^2} \left\{ \sum_{l,n=-\infty}^{\infty} (-1)^{n+l} \exp \left( i\pi n \frac{x' - x''}{2L} \right) \delta \left[ \chi_{n,l}(x,t) - \frac{x' + x''}{2L} \right] ight\} \]

It consists of four contributions, each of which involves the function

\[ D(\eta; \zeta) \equiv \sum_{m',m''=-\infty}^{\infty} \exp \left\{ i\pi (m' + m'') \eta \right\} \exp \left\{ -i\pi (m' - m'') \left[ \frac{x}{L} - (m' + m'') \frac{2T}{L} + \zeta \right] \right\}. \]  

(20)

Note that the four terms differ in the arguments of \( D \).

The function \( D \) looks rather complicated. However in the appendix we derive the equivalent representation

\[ D(\eta; \zeta) = \sum_{l,n=-\infty}^{\infty} (-1)^{n+l} e^{i\pi n \eta} \delta[\chi_{n,l}(x,t) + \zeta] \]  

(21)

where

\[ \chi_{n,l}(x,t) \equiv \frac{x}{L} - n \frac{T}{2L} - l. \]  

(22)

With the help of this relation the kernel \( K \) for the probability \( W \) to find the particle at the time \( t \) at position \( x \) reads

\[ K(x, t \mid x', x'') = \frac{1}{4L^2} \left\{ \sum_{l,n=-\infty}^{\infty} (-1)^{n+l} \exp \left( i\pi n \frac{x' - x''}{2L} \right) \delta \left[ \chi_{n,l}(x,t) - \frac{x' + x''}{2L} \right] ight\} \]

\[ + \sum_{l,n=-\infty}^{\infty} (-1)^{n+l} \exp \left( -i\pi n \frac{x' - x''}{2L} \right) \delta \left[ \chi_{n,l}(x,t) - \frac{x' + x''}{2L} \right] \]

\[ - \sum_{l,n=-\infty}^{\infty} (-1)^{n+l} \exp \left( i\pi n \frac{x' + x''}{2L} \right) \delta \left[ \chi_{n,l}(x,t) - \frac{x' - x''}{2L} \right] \]

\[ - \sum_{l,n=-\infty}^{\infty} (-1)^{n+l} \exp \left( -i\pi n \frac{x' + x''}{2L} \right) \delta \left[ \chi_{n,l}(x,t) - \frac{x' - x''}{2L} \right] \}. \]  

(23)

This is the key result of the present paper. We now discuss the properties of the kernel using this representation. Here we focus in particular on the behavior of \( K \) in the spacetime strip defined by the left and the right walls at \( x = 0 \) and \( x = L \).

We note that the kernel \( K \) has quite a characteristic form. Due to the appearance of the \( \delta \)-functions it is different from zero only along the four sets of straight spacetime lines

\[ \frac{t_{n,l}(x; x'+x'')}{T/2} = \frac{1}{n} \left( \frac{x}{L} + \frac{x' + x''}{2L} - l \right) \]  

(24)

and

\[ \frac{t_{n,l}(x; x'-x'')}{T/2} = \frac{1}{n} \left( \frac{x}{L} + \frac{x' - x''}{2L} - l \right). \]  

(25)

The steepness \( n^{-1} \) of these world lines is quantized in terms of the integer \( n \), which due to the summation can take on any value from minus infinity to plus infinity.

These lines enter or leave the spacetime strip through the left wall at \( x = 0 \) at the times

\[ \frac{t_{n,l}(x = 0; x'+x'')}{T/2} = \mp \frac{1}{n} \frac{x' + x''}{2L} - \frac{l}{n} \]  

(26)

and
\[
t_{n,l}(x = 0; x' - x'') = \frac{1}{2T} \left( x' - x'' + \frac{l}{n} \right).
\]

We note that apart from the integers \( n \) and \( l \) the integration variables \( x' \) and \( x'' \) determine these times. Hence for one set of \( n \) and \( l \) values these spacetime lines are determined by the integration variables \( x' \) and \( x'' \). However, there is a degeneracy in these lines: the integration variables \( x' \) and \( x'' \) enter these expressions either in their sum or their difference. Hence it is left to the initial wave packet to either enforce or suppress this degeneracy. This either enhances or reduces the visibility of the intermode traces, as we show in the next section.

We emphasize that there is already one degeneracy guaranteed by the quadratic energy spectrum Eq. (4) of the particle in the box: In the function \( D \) the summation indices \( m' \) and \( m'' \) enter the expression in the square brackets multiplying time in their sums \( m' + m'' \) only. Indeed by multiplying it with the prefactor \( m' - m'' \) outside of the brackets we realize that this is a consequence of the quadratic dispersion relation connecting kinetic energy and wave number. This sum \( m' + m'' \) leads eventually to the integer value \( n \) determining the steepness of the spacetime lines defined in Eq. (22). Hence many values of the summation indices \( m' \) and \( m'' \) lead to the same steepness \( n^{-1} \).

According to Eq. (23) each \( \delta \)-function has a complex valued prefactor. This prefactor contains the term \((-1)^{n-l}\) as well as the exponential \( \exp[\pm \pi n(x' - x'')/(2L)] \) or \( \exp[\pm \pi n(x' + x'')/(2L)] \). Again as in the argument of the \( \delta \)-function either the sum or the difference of the integration variables \( x' \) and \( x'' \) enters. Hence there is an interesting factorization property in \( K \): When the difference \( x' - x'' \) occurs in the argument of the \( \delta \)-functions the phase of the complex amplitude contains the sum \( x' + x'' \) and vice versa. This factorization property is essential for the emergence of the intermode traces as we discuss in Sec. IV.

We conclude this section by noting that the kernel \( K \) for the probability to find the particle at time \( t \) at the position \( x \) in the box consists of \( \delta \)-functions aligned along straight spacetime lines. These world lines have discrete steepness and enter or leave the spacetime strip at \( x = 0 \) at times determined by the sum and the difference of the integration variables \( x' \) and \( x'' \) of the initial wave packet.

\[\text{IV. EMERGENCE OF INTERMODE TRACES} \]

In the preceding section we have realized that the kernel factorizes into sums of products of two functions. Each of the functions either depends on the sum \( x' + x'' \) or the difference \( x' - x'' \) of the integration variables \( x' \) and \( x'' \), that is, of the position variables of the initial wave packet \( \varphi^*(x') \) and \( \varphi(x'') \). We are therefore lead to consider wave packets which satisfy the factorization property

\[\varphi^*(x') \varphi(x'') = \varphi_+(x' + x'') \varphi_-(x' - x'')\]

(28)

where \( \varphi_+ \) and \( \varphi_- \) are new wave functions. Moreover, the initial wave packet has to satisfy the boundary conditions. Are there any wave functions that factorize and vanish at the walls? Here we do not want to go into a full discussion of this question but only mention that a narrow Gaussian satisfies both requirements in an approximated sense as discussed in Sec. V.

For the case of factorizable wave functions we can now perform one of the two integrations with the help of the \( \delta \)-functions in the kernel \( K \). Then the probability to find the particle at time \( t \) at position \( x \) reads

\[W(x, t) = \int_0^L dx' \int_0^L dx'' \varphi_-(x' - x'') \varphi_+(x' + x'') K(x, t | x', x'').\]

(29)

Under the assumption of a very narrow initial wave packet, it is possible to extend the integration limits to minus infinity and plus infinity. Motivated by the factorization property of the kernel discussed in the preceding section we now introduce the more convenient integration variables

\[\xi_+ = \frac{1}{2L} (x' + x''),\]

(30)

and

\[\xi_- = \frac{1}{2L} (x' - x'').\]

(31)

We make use of the expression, Eq. (23), for the kernel \( K \) and the probability distribution becomes
\[ W(x,t) = \frac{1}{2} \sum_{l,n=-\infty}^{\infty} \left( -1 \right)^{n+l} \int_{-\infty}^{\infty} d\xi_+ \int_{-\infty}^{\infty} d\xi_- \varphi_- (2L\xi_-) \varphi_+ (2L\xi_+) \times \left\{ e^{i\pi n \xi_-} \delta [\chi_{n,l}(x,t) - \xi_+] + e^{-i\pi n \xi_-} \delta [\chi_{n,l}(x,t) + \xi_+] \right. \\
\left. - e^{i\pi n \xi_+} \delta [\chi_{n,l}(x,t) - \xi_-] - e^{-i\pi n \xi_+} \delta [\chi_{n,l}(x,t) + \xi_-] \right\} . \tag{32} \]

The presence of \( \delta \)-functions allows us to integrate over one variable. The remaining integral is the Fourier transform

\[ \tilde{\varphi}_{\pm} (\kappa_n) = \frac{1}{2L} \int_{-\infty}^{\infty} dy \, e^{i\kappa_n y} \varphi_{\pm} (y) \] \tag{33}

of the factorized wave packets \( \varphi_- \) and \( \varphi_+ \) to the wave number variable \( \kappa_n \equiv n\pi/(2L) \). Hence we find

\[ W(x,t) = \frac{1}{2} \sum_{l,n=-\infty}^{\infty} \left( -1 \right)^{n+l} \left\{ \tilde{\varphi}_- (\kappa_n) \varphi_+ (2L\chi_{n,l}(x,t)) + \tilde{\varphi}_- (-\kappa_n) \varphi_+ [-2L\chi_{n,l}(x,t)] \\
- \tilde{\varphi}_+ (\kappa_n) \varphi_- (2L\chi_{n,l}(x,t)) - \tilde{\varphi}_+ (-\kappa_n) \varphi_- [-2L\chi_{n,l}(x,t)] \right\}. \tag{34} \]

When we change in the second and forth term the summation over \( n \) and \( l \) by defining \( n' \equiv -n \) and \( l' \equiv -l \) and note from the definition Eq. (22) of \( \chi_{n,l} \) the relation

\[ \chi_{-n,-l}(x,t) = -\chi_{n,l}(-x,t) \] \tag{35}

we arrive at the equivalent formulation

\[ W(x,t) = \frac{1}{2} \sum_{l,n=-\infty}^{\infty} \left( -1 \right)^{n+l} \left\{ \tilde{\varphi}_- (\kappa_n) \varphi_+ (2L\chi_{n,l}(x,t)) + \varphi_+ (2L\chi_{n,l}(-x,t)) \\
- \tilde{\varphi}_+ (\kappa_n) \varphi_- (2L\chi_{n,l}(x,t)) - \varphi_- (2L\chi_{n,l}(-x,t)) \right\}. \tag{36} \]

This result is valid for any factorizable product \( \varphi^*(x') \varphi(x'') \) of initial wave packets. It brings out most clearly the way in which the initial conditions determine the visibility of the intermediate traces. Indeed, according to Eq. (36) the probability distribution \( W(x,t) \) to find the particle at time \( t \) and position \( x \) is a superposition of wave functions \( \varphi_- \) and \( \varphi_+ \), evaluated along the spacetime lines \( \chi_{n,l}(x,t) \) and \( \chi_{n,l}(-x,t) \). The slope \( n^{-1} \) of these world lines is selected by the Fourier transforms \( \tilde{\varphi}_- \) and \( \tilde{\varphi}_+ \), which represent the momentum distribution associated with the factorized wave packets. Hence, the factorized wave functions, \( \varphi_- \) and \( \varphi_+ \), and their Fourier transforms, \( \tilde{\varphi}_- \) and \( \tilde{\varphi}_+ \), play the role of weight factors for the spacetime lines \( \chi_{n,l}(x,t) \) and \( \chi_{n,l}(-x,t) \).

V. EXAMPLE

We now illustrate the result, Eq. (34), for the probability distribution \( W(x,t) \) by applying it to the special case of a Gaussian initial wave packet. Such a packet does indeed enjoy the factorization property Eq. (28). However an arbitrary Gaussian does not satisfy the boundary conditions enforced by the walls. For this reason we now focus on a Gaussian wave packet that is initially much narrower than the width of the box.

We consider a Gaussian wave packet

\[ g(x) \equiv \left( \sqrt{\pi} \Delta x \right)^{-1/2} \exp \left[ -\frac{1}{2} \left( \frac{x - \overline{x}}{\Delta x} \right)^2 \right] \exp [i\overline{p}(x - \overline{x})/\hbar] \tag{37} \]

of width \( \Delta x \) centered at \( x = \overline{x} \) and moving with average momentum \( \overline{p} \equiv \hbar \overline{k} > 0 \). Indeed this wave packet satisfies the factorization condition

\[ g^*(x') g(x'') = \varphi_+ (x' + x'') \varphi_- (x' - x'') \] \tag{38}

where the new factorized wave functions

\[ \varphi_+(y) \equiv \left( \sqrt{\pi} \Delta x \right)^{-1/2} \exp \left[ - \left( \frac{y/2 - \overline{x}}{\Delta x} \right)^2 \right] \tag{39} \]
and

$$\varphi_-(y) \equiv (\sqrt{\Delta})^{-1/2} \exp\left[-\left(\frac{y}{2\Delta x}\right)^2\right] \exp(-i\eta y/\hbar)$$

are also Gaussian wave packets.

After calculating the corresponding Fourier transforms and inserting them into Eq. (34) for the probability distribution $W(x,t)$ to find the particle at time $t$ and position $x$, one arrives at the following expression

$$W(x,t) = \frac{1}{2L} \sum_{l,n=-\infty}^{\infty} (-1)^n \left\{ \exp\left[-\left(\frac{L\chi_{n,l} - \overline{\kappa}}{\Delta x}\right)^2\right] \exp\left[-\left(\frac{\kappa_n - \overline{\kappa}}{\Delta \kappa}\right)^2\right] + \exp\left[-\left(\frac{L\chi_{n,l} + \overline{\kappa}}{\Delta x}\right)^2\right] \exp\left[-\left(\frac{\kappa_n + \overline{\kappa}}{\Delta \kappa}\right)^2\right] - 2 \exp\left[-\left(\frac{\kappa_n}{\Delta \kappa}\right)^2\right] \exp\left[-\left(\frac{L\chi_{n,l}}{\Delta x}\right)^2\right] \cos\left[2(\overline{\kappa}L\chi_{n,l} - \kappa_n\overline{\kappa})\right]\right\},$$

where $\Delta \kappa \equiv 1/\Delta x$.

We can identify in Eq. (34) two different kinds of structures among all the possible intermode traces.

We start our analysis from the Gaussian $\exp\left[-(\kappa_n - \overline{\kappa})^2/\Delta \kappa^2\right]$ which is centered around the average wave number $\overline{\kappa}$. It takes on dominant values only for $|\kappa_n - \overline{\kappa}| \sim \Delta \kappa$. The other weight factor, $\exp\left[-(L\chi_{n,l} - \overline{\kappa})^2/\Delta x^2\right]$, selects the spacetime lines starting at $t = 0$ from the initial average position $\overline{\kappa}$ of the particle in the box and from its images $\overline{\kappa} + l\chi$, periodically located along the $x$-axis. The combined effect of these two factors is to restrict the intermode traces to those connected with the classical motion. They therefore have a slope $n^{-1}$ related to the average momentum and emerge from the initial location of the particle in the potential well.

A similar argument applies to the second term of Eq. (34). In this case the spacetime lines $\chi_{n,l}(x,t)$ are characterized by a negative slope $-|n|^{-1}$ satisfying the condition $|\kappa_n + \overline{\kappa}| \sim \Delta \kappa$. They originate from $-\overline{\kappa} + l\chi$.

The third term of Eq. (34) has the form of an interference term, weighted by two Gaussians. The Gaussian containing the quantized wave number $\kappa_n$ is centered around zero. Therefore now the lines with small $n$, or equivalently with large slope $|n|^{-1}$, are enhanced. According to the weight factor $\exp\left[-(L\chi_{n,l}/\Delta x)^2\right]$ these structures emerge at the time $t = 0$ from the walls of the box, located at $x = 0$ and $x = L$, and from their replicas periodically placed at $x = lL$. These are indeed the relevant intermode traces giving rise to the regular pattern in the spacetime plot of the probability distribution $W(x,t)$.

The last factor, $\cos\left[2(\overline{\kappa}L\chi_{n,l} - \kappa_n\overline{\kappa})\right]$, provides a modulation depending on the initial conditions, that is average position and wave number. In the extreme case of zero momentum, shown in Fig. 1, the cosine factor reduces to $\cos(n\pi\overline{\kappa}/L)$. Hence whenever its argument is equal to $\pm \pi/2 \mod(2\pi)$ the corresponding intermode traces are washed out. Indeed, in the example considered in Fig. 1 the lines $t/(T/2) = \pm 1/2(x/L - l)$ are not present because the cosine factor $\cos(n\pi/4)$ vanishes for $n = \pm 2$.

FIG. 1. Density plot of the probability distribution $W(x,t)$ to find the particle at time $t$ at position $x$. The initial wave packet is a Gaussian with width $\Delta x = L/20$ and average wave number $\overline{\kappa} = 0$ centered at $\overline{\kappa} = L/4$. Darker areas correspond to minima of probability, while brighter ones represent maxima.
In the opposite limit of large average momentum, the cosine term is responsible for the fine structure of the quantum carpet. A comparison between Figs. 1 and 2 shows that by increasing the initial momentum, both canals and ridges develop neighboring structures: Consider, for example, the lines running along the main diagonals. In the case of non-vanishing initial wave numbers they split into an alternating series of canals and ridges. The detailed spatial behavior of such intermode traces is shown on top of Fig. 2.

FIG. 2. Density plot of the probability distribution of the particle in a box as a function of position and time. The initial wave function is a Gaussian of width $\Delta x = L/20$ and average wave number $k = 20\pi/L$ centered at $x = L/4$. On top we show a magnified view of the interference term in Eq. (41) for $n = 1$, that is for the diagonal connecting the lower left corner and the upper right corner, and for the other main diagonal corresponding to $n = -1$. Note that in the first case two ridges surround a canal, while in the second case the situation is reversed and two canals surround a ridge.

VI. CONCLUSIONS

We have studied the probability distribution of a particle in a one-dimensional box as a function of position and time. The corresponding density plot in spacetime is characterized by a regular pattern of intermode traces, that is canals or ridges cutting through and building onto an almost uniform background of probability.

In order to explain this phenomenon we have related the probability distribution to the product of the initial wave packet and its complex conjugate via the kernel $K$. This formulation allows us to distinguish between the intrinsic characteristics of the system and the influence of the specific initial conditions.

Indeed we have found that the kernel, which consists of the product of two Green’s functions, contains already the spacetime structures. It can be expressed as a superposition of $\delta$-functions whose argument is a linear function of time and position. The kernel is non-vanishing only along this set of infinitely many lines with discrete steepness. However, the initial conditions can either enhance or suppress the visibility of such structures. They therefore select the ones with the largest degeneracy from all possible intermode traces.

We have shown that an initial wave packet which satisfies a certain factorization property is especially suitable to bring out the pattern in the probability distribution. An example of such wave functions is the Gaussian wave packet, discussed here. We emphasize however that the treatment presented here is more general. It even allows us to
investigate the case of a uniform initial distribution with discontinuities, analyzed by Berry in the context of fractal properties of the spacetime probability distribution.

ACKNOWLEDGEMENT

We express our gratitude to P. J. Bardroff, M. V. Berry, M. Fontenelle, F. Großmann, M. Hall, T. Kiss, W. E. Lamb, Jr., K. A. H. van Leeuwen, C. Leichtle, J. Marklof, M. M. Nieto, J. M. Rost, F. Saïf and P. Stifter for many fruitful discussions on this topic. One of us (I. M.) thanks the organizers of this conference for the opportunity to report this work and for a most splendid meeting. Two of us (I. B.-B.) and (A. E. K.) thank the Humboldt Stiftung for their support.

APPENDIX: NEW REPRESENTATION OF $D$

In this appendix we reexpress the function $D(\eta; \zeta) \equiv \sum_{m', m'' = -\infty}^{\infty} \exp[i\pi (m' + m'') \eta] \exp\{-i\pi (m' - m'') [\xi - (m' + m'')2\tau + \zeta]\}$

\begin{equation}
D(\eta; \zeta) = \sum_{m', m'' = -\infty}^{\infty} \exp[i\pi (m' + m'') \eta] \exp\{-i\pi (m' - m'') [\xi - (m' + m'')2\tau + \zeta]\}
\end{equation}

defining the kernel $K$, Eq. (19), in terms of infinitely many $\delta$-functions aligned along straight lines in spacetime. Throughout this appendix we use the dimensionless position variables $\xi, \eta$ and $\zeta$ normalized to the length of the box and the dimensionless time $\tau$ scaled with respect to the revival time $T$.

We note from the definition of $D$ that only the sum $m' + m''$ and the difference $m' - m''$ of the summation indices $m'$ and $m''$ occur. This suggests to introduce new summation indices $m \equiv m' + m''$ and $k \equiv m' - m''$. However, this definition implies that $m' = (k + m)/2$ and $m'' = (m - k)/2$. Hence when one of the two new indices is odd and the other is even the quantities $m'$ and $m''$ are not integer anymore. Therefore, $m$ and $k$ must both be either even or odd leading to the substitutions

\begin{equation}
2m = m' + m'' \quad \text{and} \quad 2k = m' - m''
\end{equation}

or

\begin{equation}
2m + 1 = m' + m'' \quad \text{and} \quad 2k + 1 = m' - m''
\end{equation}

and to the representation

\begin{equation}
D = \sum_{k, m = -\infty}^{\infty} e^{i\pi (2m) \eta} \exp\{-i\pi (2k) [\xi - (2m)2\tau + \zeta]\}
\end{equation}

\begin{equation}
+ \sum_{k, m = -\infty}^{\infty} e^{i\pi (2m + 1) \eta} \exp\{-i\pi [\xi - (2m + 1)2\tau + \zeta]\} \exp\{-i\pi (2k) [\xi - (2m + 1)2\tau + \zeta]\}.
\end{equation}

When we recall the relation

\begin{equation}
\sum_{k = -\infty}^{\infty} \exp(-2\pi ik\theta) = \sum_{l = -\infty}^{\infty} \delta(\theta - l)
\end{equation}

we can perform the summation over $k$ and arrive at

\begin{equation}
D = \sum_{l, m = -\infty}^{\infty} e^{i\pi (2m) \eta} \delta[\xi - (2m)2\tau + \zeta - l]
\end{equation}

\begin{equation}
+ \sum_{l, m = -\infty}^{\infty} e^{i\pi (2m + 1) \eta} \exp\{-i\pi [\xi - (2m + 1)2\tau + \zeta]\} \delta[\xi - (2m + 1)2\tau + \zeta - l]
\end{equation}

which with the help of
\begin{equation}
f(\xi) \delta(\xi) = f(0) \delta(\xi) \tag{48}
\end{equation}

simplifies to

\begin{equation}
D = \sum_{l,m=-\infty}^{\infty} e^{i\pi(2m)\eta} \delta[\xi - (2m)2\tau + \zeta - l] \\
+ \sum_{l,m=-\infty}^{\infty} e^{i\pi(2m+1)\eta} e^{-i\pi l} \delta[\xi - (2m + 1)2\tau + \zeta - l]. \tag{49}
\end{equation}

We can combine the sum over \((2m)\) and the one over \((2m + 1)\) into one sum over \(n\) when we recall the relation

\begin{equation}
e^{-i\pi l} = (-1)^l \tag{50}
\end{equation}

and note that

\begin{equation}
(-1)^n l = \begin{cases}
1 & \text{for } n = 2m \\
(-1)^l & \text{for } n = 2m + 1.
\end{cases} \tag{51}
\end{equation}

This yields the new representation

\begin{equation}
D(\eta; \zeta) = \sum_{n,l=-\infty}^{\infty} (-1)^n l e^{i\pi n\eta} \delta[\xi - n(2\tau) + \zeta - l] \tag{52}
\end{equation}

which is central to the analysis of the kernel \(K\) in Sec. III.

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