Huygens-Fresnel-Kirchhoff construction for quantum propagators with application to diffraction in space and time

Arseni Goussev
Max Planck Institute for the Physics of Complex Systems, Nöthnitzer Straße 38, D-01187 Dresden, Germany

(Dated: January 9, 2012)

We address the phenomenon of diffraction of non-relativistic matter waves on openings in absorbing screens. To this end, we expand the full quantum propagator, connecting two points on the opposite sides of the screen, in terms of the free particle propagator and spatio-temporal properties of the opening. Our construction, based on the Huygens-Fresnel principle, describes the quantum phenomena of diffraction in space and diffraction in time, as well as the interplay between the two. We illustrate the method by calculating diffraction patterns for localized wave packets passing through various time-dependent openings in one and two spatial dimensions.

PACS numbers: 03.65.Nk, 03.75.-b, 42.25.Fx

I. INTRODUCTION

Diffraction and interference of matter are among the most fascinating and controversial aspects of quantum theory. It is not surprising that laboratory exploration of these phenomena with subatomic, atomic, and molecular particles has been at the heart of experimental research since early days of quantum mechanics [1]. As of today, a wave-like behavior of matter has been successfully demonstrated for a number of elementary particles, atoms, simple molecules (see Ref. [1] for a comprehensive review), and, most notably, for some heavy organic compounds including C_{60} [2], C_{70} [3], and $C_{60}F_{48}$ [4]. A majority of these experiments involve sending a mono-energetic beam of particles through a screen with openings (apertures) such as slits, diffraction gratings, or Fresnel zone plates. Mathematically, the problem of quantum diffraction on stationary spatial apertures can be described by the Poisson equation and treated by methods originally developed in the context of diffraction and interference of light [5, 6].

A diffraction phenomenon of a different kind – "diffraction in time" – was introduced by Moshinsky six decades ago [7] and subsequently studied by many researchers, both experimentally [8] and theoretically (see Refs. [9, 10] for reviews). The phenomenon has to do with time evolution (more precisely, with non-uniform spreading) of initially sharp wave fronts in quantum systems, and manifests itself already in one dimension. Thus, in the original set-up proposed by Moshinsky [7], a perfectly absorbing shutter is placed in the way of a mono-energetic beam of non-relativistic quantum particles. Then, a sudden removal of the shutter creates a "chopped" particle beam with a sharp wave front. As shown by Moshinsky, such a wave front disperses non-uniformly in the course of time and, most interestingly, develops a sequence of diffraction fringes. Mathematically, these fringes appear to be analogous to the ones observed in diffraction of light on the edge of a semi-infinite plane.

There are several ways of treating quantum diffraction theoretically. One commonly used, physically motivated method for evaluating the wave function of a quantum particle passing through an opening in a diffraction screen is the "truncation" approximation, which is based on the composition property of quantum propagators. In this approximation, transmission of a spatially localized wave packet through the diffraction screen is treated as a three stage process: (i) the wave packet is propagated freely during the time that it takes the corresponding classical particle to reach the screen, then (ii) the wave function is reshaped (or truncated) in accordance with the geometry of the aperture, and, finally, (iii) the resultant wave function is propagated freely for the remaining time interval. The reader is referred to Refs. [11–14] for details and implementation examples of the truncation approximation.

One drawback of the truncation approximation is that it does not account for diffraction in time. Brukner and Zeilinger [15] proposed another, more versatile method for solving the problem of quantum diffraction. The central assumption of their method is that the time-dependent wave function in question satisfies certain explicitly known, inhomogeneous time-dependent Dirichlet boundary conditions at the surface of the diffraction screen. More specifically, two assumptions are made: (i) the value of the wave function at a point inside the aperture is assumed to equal the value that the wave function would have at this point if the diffraction screen was absent, and (ii) the wave function vanishes at every point of the diffraction screen outside the aperture. The first assumption is commonly referred to as the Kirchhoff approximation, while the second corresponds to the physical assumption of *perfect reflectivity* of the screen. The method of Brukner and Zeilinger has since been successfully used by several researchers to study quantum diffraction in both space and time [16–18].

In this paper, we present another approach to quantum diffraction in space and time. Our method is based on the Huygens-Fresnel principle and Kirchhoff theory of diffraction, and allows one to calculate the time-dependent quantum propagator for the problem of particle diffraction on spatio-temporal openings in otherwise *perfectly absorbing* screens. Our expression for the propagator is especially adaptable for calculating diffraction patterns in situations in which the initial wave function is given by a spatially localized wave packet or by a superposition of several localized wave packets. Similar to the method of Brukner and Zeilinger, our construction provides a unified framework that treats the phenomena of diffraction in space and diffraction in time on the same footage. The main difference between the method of Brukner and Zeilinger and our method is that the former is designed to treat perfectly reflecting screens, while the latter is only applicable to perfectly absorbing ones. Finally, our approach allows for calculation of quantum diffraction patterns produced by openings in spatially curved screens.

The paper is organized as follows. In Sec. II we develop an expansion of the propagator for a non-relativistic quantum particle passing through a time-dependent opening in an absorbing screen. In Sec. III we demonstrate utility of the expansion by applying it to some example systems in one and two spatial dimensions. In Sec. IV we discuss our results and make concluding remarks. Some technicalities are deferred to an Appendix.

II. HUYGENS-FRESNEL-KIRCHHOFF CONSTRUCTION FOR QUANTUM PROPAGATORS

In this section, we address two quantum-mechanical phenomena – diffraction in time, pioneered by Moshinsky [7, 9, 10], and diffraction in space, as described by Kirchhoff theory [5, 6]. We recast standard descriptions of both phenomena in a way analogous to a time-dependent formulation of the Huygens-Fresnel principle. Expressed in this way, the two diffraction processes appear to be closely related and can be straightforwardly unified into a single model of diffraction in space and time.

A. Notation

In order to facilitate the clarity of the following presentation, we begin by introducing central physical quantities and fixing notation.

The focus of this paper is on the quantum propagator $K(\mathbf{q},\mathbf{q}';t)$ that describes the motion of a quantum particle in the f-dimensional coordinate space by relating a particle's wave function $\Psi(\mathbf{q};t)$ at time t to that at time $t=0$ through

$$\Psi(\mathbf{q};t) = \int_{\mathbb{R}^f} \mathrm{d}^f\mathbf{q}'\, K(\mathbf{q},\mathbf{q}';t)\Psi(\mathbf{q}';0)\,. \tag{1}$$

The propagator is the solution of the time-dependent Schrödinger equation

$$i\hbar\frac{\partial K}{\partial t} = H_{\mathbf{q}}K \tag{2}$$

with the initial condition

$$\lim_{t\to 0} K(\mathbf{q},\mathbf{q}';t) = \delta(\mathbf{q}-\mathbf{q}')\,, \tag{3}$$

where $H_{\mathbf{q}}$ denotes the Hamilton operator in the position representation. (The propagator is also subject to certain absorbing boundary conditions that we do not discuss at this point.) In the case of a free particle of mass m we have $H_{\mathbf{q}} = -\frac{\hbar^2}{2m}\boldsymbol{\nabla}^2_{\mathbf{q}}$ and $K = K_0(\mathbf{q}-\mathbf{q}';t)$ with

$$K_0(\mathbf{q}-\mathbf{q}';t) = \left(\frac{m}{2\pi i\hbar t}\right)^{\frac{f}{2}} \exp\left(-\frac{m|\mathbf{q}-\mathbf{q}'|^2}{2i\hbar t}\right)\,. \tag{4}$$

Hereinafter, the subscript "$_0$" indicates that the corresponding quantity refers to the case of a free particle.

We also consider the energy-domain Green function defined as the Laplace transform of the propagator,

$$\begin{aligned} G(\mathbf{q},\mathbf{q}';E) &= \int_0^\infty \mathrm{d}t\, \mathrm{e}^{-st} K(\mathbf{q},\mathbf{q}';t) \\ &\equiv \mathcal{L}[K](\mathbf{q},\mathbf{q}';s) \quad \text{with} \quad s = \frac{E}{i\hbar}\,. \end{aligned} \tag{5}$$

Consequently, the propagator is obtained from the Green function by means of the inverse Laplace transform, $K = \mathcal{L}^{-1}[G]$. In the free particle case, Eqs. (4) and (5) define the free-particle Green function $G_0(\mathbf{q}-\mathbf{q}';E) = \mathcal{L}[K_0](\mathbf{q}-\mathbf{q}';s)$ that satisfies

$$\boldsymbol{\nabla}^2_{\mathbf{q}}G_0 + k^2G_0 = -\frac{2m}{i\hbar}\delta(\mathbf{q}-\mathbf{q}') \quad \text{with} \quad k^2 = \frac{2mE}{\hbar^2}\,. \tag{6}$$

B. Diffraction in time

We now address the phenomenon of diffraction in time, first considered by Moshinsky [7] and later explored by many researchers (see Refs. [9, 10] for reviews). In its one-dimensional formulation, the Moshinsky problem is concerned with time evolution of a quantum particle, whose wave function $\Psi(\xi;t)$ is localized to the semi-infinite interval $(-\infty, x_1)$ at time $t=0$, i.e., $\Psi(\xi;0)=0$ for $\xi > x_1$. Over time, an absorbing wall (shutter) is switched "on" and "off" at the point x_1, according to a protocol defined by a characteristic function $\chi(t)$. The latter is allowed to take values between 0 and 1, with 0 representing the case of perfect absorption (shutter "on") and 1 corresponding to perfect transmission (shutter "off"). The open interval $0 < \chi < 1$ represents the case of partially absorbing and partially transmitting (but reflection-free) shutter. One is then interested in the wave function $\Psi(\xi;t)$ of the particle to the right of the shutter, $\xi > x_1$, at $t > 0$. Moshinsky [7] analyzed this problem for a "monochromatic" incident wave $\Psi(\xi;0) = \Theta(x_1-\xi)\mathrm{e}^{ik\xi}$, where $k > 0$ and Θ is the Heaviside step function, and a perfectly absorbing shutter that gets suddenly removed at an instant t_0, i.e., $\chi(t) = \Theta(t-t_0)$. His analysis showed that at times $t > t_0$, the front of the probability density wave exhibits patterns identical to those observed in the Fresnel diffraction of light from the edge of a semi-infinite plane, thus giving rise to the term "diffraction in time".

Our objective is to devise an expression for the propagator $K(x, x'; t)$ that describes Moshinsky diffraction by a shutter positioned at a point x_1, such that

$$x' < x_1 < x \,, \tag{7}$$

and controlled (opened and closed) in accordance with the characteristic function $\chi(t)$ of an arbitrary functional form. Our construction relies on the Huygens-Fresnel principle, which, for the purpose of the current problem, can be formulated as follows: The disturbance at the point x produced by a source O', located at some other point x', can be viewed as produced by a fictitious source O_1, located at a point x_1 in between x' and x, cf. Eq. (7). The strength of the fictitious source O_1 is determined by the disturbance at the point x_1 produced by the original source O'. When a (partially) absorbing shutter is placed at the point x_1, the strength of the fictitious source O_1 is modulated by the characteristic function $\chi(t)$ taking values between 0 and 1. Mathematically, this can be summarized as

$$\begin{aligned} K(x, x'; t) = & \int_0^t \mathrm{d}t_1 \, u(x - x_1, x_1 - x'; t, t_1) \\ & \times K_0(x - x_1; t - t_1)\chi(t_1)K_0(x_1 - x'; t_1) \,. \end{aligned} \tag{8}$$

where u, having dimensions of speed, is a yet-to-be-determined function of the distances $x - x_1$ and $x_1 - x'$ and times t and t_1.

The physical meaning of Eq. (8) is transparent: The probability amplitude of an event in which the particle goes from x' to x in time t can be expressed as a sum of probability amplitudes over all composite events in which the particle first goes from x' to an intermediate point x_1 in a time t_1 and then reaches x from x_1 in the remaining time $t - t_1$. Because of their simple physical interpretation, propagator expansions similar to Eq. (8) are often used for qualitative description of quantum interference phenomena (e.g., see [9] for a qualitative discussion of a two-slit interference experiment), however the explicit functional form of u is usually neither specified nor taken into account.

1. *Free particle,* $\chi(t) = 1$

Interested in determining the functional form of $u = u(x - x_1, x_1 - x'; t, t_1)$, we first direct our attention to the simplest possible scenario, in which the shutter stays open throughout the entire time interval from 0 to t, i.e., $\chi(t_1) = 1$ for $0 \le t_1 \le t$. In this case, the propagator in the left-hand side of Eq. (8) is given by the free particle propagator, $K = K_0$, requiring u to satisfy

$$K_0(x - x'; t) = \int_0^t \mathrm{d}t_1 \, u \, K_0(x - x_1; t - t_1)K_0(x_1 - x'; t_1) \,. \tag{9}$$

It is interesting to observe that Eq. (9) does not specify the function u uniquely. In fact, Eq. (9) turns out to be an identity satisfied exactly by infinitely many different functions u, some examples being (see App. A)

$$u = \eta \frac{x - x_1}{t - t_1} + (1 - \eta)\frac{x_1 - x'}{t_1} \,, \tag{10}$$

$$u = \sqrt{\frac{2i\hbar}{\pi m t}} \frac{\exp(-\zeta^2)}{\operatorname{erfc}(\zeta)} \quad \text{with} \quad \zeta^2 = \frac{m(x - x')^2}{2i\hbar t} \,. \tag{11}$$

Here, η is an arbitrary complex number, and "erfc" denotes the complementary error function.

2. *Moshinsky shutter,* $\chi(t) = \Theta(t - t_0)$

We now show that the functional form of u can be uniquely determined by comparing Eq. (8) with an exact expression for the quantum propagator in the original Moshinsky set-up [7], in which the absorbing shutter, located at x_1, is closed until a time t_0 and open afterwards, i.e., $\chi(t_1) = \Theta(t_1 - t_0)$ for $0 \le t_0, t_1 \le t$.

On one hand, a direct construction of the propagator $\widetilde{K}_{\mathrm{M}}(x, x'; t)$ for the original Moshinsky problem leads to

$$\begin{aligned} \widetilde{K}_{\mathrm{M}}(x, x'; t) &= \int_{-\infty}^{x_1} \mathrm{d}x'' \, K_0(x - x''; t - t_0)K_0(x'' - x'; t_0) \\ &= K_0(x - x'; t) \left[1 - \frac{1}{2}\operatorname{erfc}\left((x_1 - x_0)\sqrt{\frac{mt}{2i\hbar t_0(t - t_0)}}\right)\right] \end{aligned} \tag{12}$$

with

$$x_0 = x\frac{t_0}{t} + x'\frac{t - t_0}{t} \,. \tag{13}$$

The first equality in Eq. (12) combines the composition property of quantum propagators and the fact that, at time t_0, all the probability density to the right of x_1 has been absorbed by the shutter. This leads to the truncation of the upper limit in the x'' integral.

On the other hand, a substitution of $\chi(t_1) = \Theta(t_1 - t_0)$ into Eq. (8) yields

$$\begin{aligned} K_{\mathrm{M}}(x, x'; t) = & \int_{t_0}^t \mathrm{d}t_1 \, u(x - x_1, x_1 - x'; t, t_1) \\ & \times K_0(x - x_1; t - t_1)K_0(x_1 - x'; t_1) \,. \end{aligned} \tag{14}$$

Equations (12) and (14) allow us to uniquely determine the function form of u by requiring $\widetilde{K}_{\mathrm{M}} = K_{\mathrm{M}}$. Indeed, let us for the moment fix the values of x, x', and t, and treat the propagator $\widetilde{K}_{\mathrm{M}}$ as a function of the shutter opening time t_0 only, i.e., $\widetilde{K}_{\mathrm{M}} = \widetilde{K}_{\mathrm{M}}(t_0)$. First, we note that $\lim_{t_0 \to t^-} \widetilde{K}_{\mathrm{M}} = 0$. Indeed, $x_0 \to x$ as $t_0 \to t^-$, and the argument of the complementary error function in Eq. (12) tends to $\mathrm{e}^{i3\pi/4}\infty$, making the value of the complementary error function approach 2. This limit, of course, corresponds to the trivial case of the absorbing shutter being closed throughout the entire time interval from 0 to t. Then, in view of this limit, we rewrite the Moshinsky propagator as

$$\widetilde{K}_{\mathrm{M}}(t_0) = -\int_{t_0}^{t} \mathrm{d}t_1 \, \frac{\mathrm{d}\widetilde{K}_{\mathrm{M}}(t_1)}{\mathrm{d}t_1} \,. \tag{15}$$

A straightforward (but somewhat tedious) calculation yields

$$\frac{\mathrm{d}\widetilde{K}_{\mathrm{M}}(t_1)}{\mathrm{d}t_1} = -\frac{1}{2}\left(\frac{x - x_1}{t - t_1} + \frac{x_1 - x'}{t_1}\right) \times K_0(x - x_1; t - t_1) K_0(x_1 - x'; t_1) \,. \tag{16}$$

It is now clear that the Moshinsky propagator $\widetilde{K}_{\mathrm{M}}$, as expressed by Eqs. (15) and (16), is equivalent to the propagator K_{M}, given by Eq. (14) with

$$u = \frac{1}{2}\left(\frac{x - x_1}{t - t_1} + \frac{x_1 - x'}{t_1}\right) \,. \tag{17}$$

Note that Eq. (17) is equivalent to Eq. (10) with $\eta = 1/2$. Also, Eq. (17) provides the physical meaning of the function u: The latter is a characteristic (mean) velocity of the particle when it traverses the shutter.

3. *Arbitrary* $\chi(t)$

A substitution of Eq. (17) into Eq. (8) yields

$$K(x, x'; t) = \frac{1}{2}\int_0^{t} \mathrm{d}t_1 \left(\frac{x - x_1}{t - t_1} + \frac{x_1 - x'}{t_1}\right) \times K_0(x - x_1; t - t_1) \chi(t_1) K_0(x_1 - x'; t_1) \,. \tag{18}$$

Here, the spatial points x, x', and x_1 are subject to the condition given by Eq. (7), and the characteristic function χ is allowed to take values between 0 (perfect absorption) and 1 (perfect transmission).

Equation (18) provides a formulation of the Huygens-Fresnel principle for a one-dimensional particle in the presence of a point-like absorbing obstacle, whose absorbing properties change in the course of time. At this point, it is important to emphasize that the analysis provided in this section should not be regarded as a rigorous mathematical proof of the propagator expansion (18). Unavoidable difficulties in solving the problem from the first principles stem from the lack of a proper unambiguous definition of point-like, generally partial and time-dependent, absorption. In our approach, however, we bypass this issue by modeling the absorption with the help of a time-dependent characteristic function, $\chi(t)$, and relying on the validity of the Huygens-Fresnel construction in its most general form, Eq. (8). Consequently, we remove any arbitrariness in the Huygens-Fresnel construction by determining the function u, originally unknown in Eq. (8), through analyzing the case of $\chi(t)$ corresponding to the Moshinsky shutter problem, for which point-like absorption can be defined unambiguously.

It is interesting to note a formal similarity between Eq. (18) and the well-known Lippmann-Schwinger equation [9, 11, 19], which in the case of a point-like perturbation, situated at x_1 and described by a spatio-temporal potential of the form $V(\xi, \tau) = \delta(\xi - x_1) U(\tau)$, reads

$$K_{\mathrm{sc}}(x, x'; t) = K_0(x - x'; t) - \frac{i}{\hbar}\int_0^{t} \mathrm{d}t_1 \, K_0(x - x_1; t - t_1) U(t_1) K_{\mathrm{sc}}(x_1, x'; t_1) \,. \tag{19}$$

As before, K_0 is the (free-particle) propagator in the absence of the perturbation potential, and K_{sc} is the propagator corresponding to the full scattering problem. Equation (19) gives rise to a multiple collision representation of the scattering propagator, known as the Dyson series [11, 19].

Despite their superficial resemblance, Eqs. (18) and (19) describe very different physical processes: The Lippmann-Schwinger equation pertains to the phenomenon of quantum scattering, whereas the Huygens-Fresnel propagator expansion represents quantum motion in the presence of obstacles that (partially) absorb matter waves without deflecting them. In fact, it is easy to show that the Lippmann-Schwinger equation can not be used to model perfect absorption, corresponding to the trivial choice $\chi = 0$ in Eq. (18). Indeed, the case of a perfectly absorbing obstacle at x_1 would require $K_{\mathrm{sc}}(\xi, x'; t) = \Theta(x_1 - \xi) K_0(\xi - x'; t)$, which is clearly incompatible with Eq. (19).

In order to avoid possible confusion, we emphasize that it is the assumption of a point-like perturbation, $V(\xi, \tau) = \delta(\xi - x_1) U(\tau)$, that does not allow the Lippmann-Schwinger equation to properly capture the physics of absorption. On the opposite, the Lippmann-Schwinger equation with a smooth, complex-valued potential function $V(\xi, \tau)$, defined over an extended spatial interval, is often the method of choice in modeling absorbing boundaries (see Ref. [20] for a comprehensive review).

4. *Continuously opening shutter,* $\chi(t) = \mathrm{e}^{-\tau/t}$

In order to demonstrate the usefulness of the Huygens-Fresnel formulation of diffraction in time we apply the propagator expansion (18) to a modified Moshinsky shutter problem, in which the absorbing shutter is initially closed, $\chi(t_1) = 0$ for $t_1 \le 0$, and then opens continuously in accordance with

$$\chi(t_1) = \exp(-\tau/t_1) \quad \text{for} \quad t_1 > 0 \,. \tag{20}$$

Here, $\tau > 0$ determines the rate at which the shutter opens. Note that the shutter described by Eq. (20) is completely removed only in the limit of infinitely long times, $\lim_{t_1 \to +\infty} \chi(t_1) = 1$.

Using the Huygens-Fresnel expansion (18), we now derive an explicit expression for the propagator $K(x, x'; t)$ connecting a point x' to the left of the shutter ($x' < x_1$) at time 0 with another point x to the right of the shutter ($x_1 < x$) at time t. To this end, we rewrite Eq. (18), in view of Eq. (4), as

$$K(x, x'; t) = -\frac{i\hbar}{2m}\left(\frac{\partial}{\partial x} - \frac{\partial}{\partial x'}\right) \int_0^t \mathrm{d}t_1 K_0(x - x_1; t - t_1)\chi(t_1)K_0(x_1 - x'; t_1)\,. \quad (21)$$

Then, taking into account Eq. (20), we write $\chi(t_1)K_0(x_1 - x'; t_1) = K_0(x_1 - \tilde{x}; t_1)$, where $\tilde{x}$ satisfies

$$(x_1 - \tilde{x})^2 = (x_1 - x')^2 + \frac{2i\hbar\tau}{m}\,. \quad (22)$$

Solving Eq. (22) for $\tilde{x}$ and choosing the solution that converges to x' in the limit $\tau \to 0^+$, we have

$$\tilde{x} = x_1 - \rho \mathrm{e}^{i\theta}\,, \quad (23)$$

where

$$\rho = \left[(x_1 - x')^4 + \left(\frac{2\hbar\tau}{m}\right)^2\right]^{\frac{1}{4}}, \quad (24)$$

$$\theta = \frac{1}{2}\tan^{-1}\frac{2\hbar\tau}{m(x_1 - x')^2}\,. \quad (25)$$

Equation (21) can now be rewritten as

$$K(x, x'; t) = -\frac{i\hbar}{2m}\left(\frac{\partial}{\partial x} - \frac{\partial\tilde{x}}{\partial x'}\frac{\partial}{\partial\tilde{x}}\right) \int_0^t \mathrm{d}t_1 K_0(x - x_1; t - t_1)K_0(x_1 - \tilde{x}; t_1)\,. \quad (26)$$

The integral over t_1 can now be evaluated explicitly:

$$\int_0^t \mathrm{d}t_1 K_0(x - x_1; t - t_1)K_0(x_1 - \tilde{x}; t_1) = \frac{m}{2i\hbar}\,\mathrm{erfc}\left(\sqrt{\frac{m}{2i\hbar t}}(x - \tilde{x})\right)\,. \quad (27)$$

This identity is derived in Appendix A for the case of real-valued $\tilde{x}$ (see Eqs. (A2) and (A7)); the derivation however can be extended to the case of $\mathrm{Re}\,\tilde{x} < x_1 < x$ and $\mathrm{Im}\,\tilde{x} \le 0$ (cf. Eqs. (23-25)). Finally, substituting Eq. (27), together with $\partial\tilde{x}/\partial x' = (x_1 - x')/(x_1 - \tilde{x})$, into Eq. (26) and taking the partial derivatives with respect to x and $\tilde{x}$, we arrive at

$$K(x, x'; t) = \frac{1}{2}\left(1 + \frac{x_1 - x'}{x_1 - \tilde{x}}\right)K_0(x - \tilde{x}; t)\,. \quad (28)$$

Two quick remarks are in order. First, Eq. (28) guaranties that, as expected, $K(x, x'; t) \to K_0(x - x'; t)$ as $\tau \to 0^+$. This limit corresponds to the standard Moshinsky set-up in which the shutter stays completely open at $t > 0$. Second, it is clear from Eq. (28) that the propagator $K(x, x'; t)$ is not symmetric in the coordinates x and x'. The absence of such symmetry is typical for quantum motion in the presence of time-dependent obstacles (e.g., see Sec. A.1 in Ref. [9]).

C. Diffraction in space

We now address Kirchhoff theory of diffraction in space [5, 6]. In particular, we rewrite the Kirchhoff's formulation in its time-dependent form, in which it can be directly applied to diffraction of quantum wave packets.

To this end, we consider a smooth $(f-1)$-dimensional surface S that is defined as the zero set of a real-valued function $s : \mathbb{R}^f \to \mathbb{R}$,

$$S = \{\mathbf{q}_1 \in \mathbb{R}^f \,:\, s(\mathbf{q}_1) = 0\}\,. \quad (29)$$

The surface S is assumed to partition the position space into two disjoint regions, such that the function s takes different (and constant) signs in the two regions. We also consider two spatial points, $\mathbf{q}$ and $\mathbf{q'}$, that lie on the opposite sides of the surface. For concreteness we take $s(\mathbf{q}) > 0$ and $s(\mathbf{q'}) < 0$. The surface S gives the location of a non-transparent, absorbing screen, in which some transparent openings (apertures) may be "cut out". These openings and, more generally, the absorbing properties of the screen, can be described by a spatially-dependent characteristic function $\chi(\mathbf{q}_1)$ taking values between zero (perfect absorption) and one (perfect transmission) at a point $\mathbf{q}_1 \in S$. Kirchhoff theory of diffraction [5, 6] allows one to express the Green function $G(\mathbf{q}, \mathbf{q'}; E)$, connecting the points $\mathbf{q}$ and $\mathbf{q'}$ at an energy E, as an integral along the screen:

$$G(\mathbf{q}, \mathbf{q'}; E) = -\frac{i\hbar}{2m}\int_{\mathbb{R}^f} \mathrm{d}^f\mathbf{q}_1\,\delta\big(s(\mathbf{q}_1)\big)\chi(\mathbf{q}_1) \times \boldsymbol{\nabla}s(\mathbf{q}_1)\cdot\Big(G_0(\mathbf{q} - \mathbf{q}_1; E)\boldsymbol{\nabla}_{\mathbf{q}_1}G_0(\mathbf{q}_1 - \mathbf{q'}; E) - G_0(\mathbf{q}_1 - \mathbf{q'}; E)\boldsymbol{\nabla}_{\mathbf{q}_1}G_0(\mathbf{q} - \mathbf{q}_1; E)\Big)\,. \quad (30)$$

It is important to emphasize that Kirchhoff method, Eq. (30), is not applicable to diffraction on apertures in transmission screens with reflecting (e.g., Dirichlet or Neumann) boundary conditions. Instead, Kirchhoff theory is known to be a good model for diffraction on perfectly absorbing, or "black", infinitely thin obstacles [21–23]. In fact, Eq. (30) provides an exact solution to the time-independent diffraction problem with the boundary conditions on the screen given by the so-called Kottler discontinuity (see Refs. [22, 23] and references within): The probability amplitude field has a discontinuity across the screen equal to minus the value of the free-space field at that point. A similar condition is imposed on the normal derivative of the field.

For our purposes, it is important to construct a time-dependent formulation of Kirchhoff diffraction. This is straightforwardly achieved by first rewriting Eq. (30) as

$$G(\mathbf{q},\mathbf{q}';E) = -\frac{i\hbar}{2m}\int_{\mathbb{R}^f} \mathrm{d}^f\mathbf{q}_1\,\delta\big(s(\mathbf{q}_1)\big)\chi(\mathbf{q}_1) \\ \times \boldsymbol{\nabla}s(\mathbf{q}_1)\cdot(\boldsymbol{\nabla}_{\mathbf{q}}-\boldsymbol{\nabla}_{\mathbf{q}'})\,G_0(\mathbf{q}-\mathbf{q}_1;E)G_0(\mathbf{q}_1-\mathbf{q}';E)\,, \tag{31}$$

and then performing the inverse Laplace transform from energy-dependent Green functions to time-dependent propagators, yielding

$$K(\mathbf{q},\mathbf{q}';t) = \frac{1}{2}\int_0^t \mathrm{d}t_1\int_{\mathbb{R}^f}\mathrm{d}^f\mathbf{q}_1\,\delta\big(s(\mathbf{q}_1)\big) \\ \times\left(\frac{\mathbf{q}-\mathbf{q}_1}{t-t_1}+\frac{\mathbf{q}_1-\mathbf{q}'}{t_1}\right)\cdot\boldsymbol{\nabla}s(\mathbf{q}_1) \\ \times K_0(\mathbf{q}-\mathbf{q}_1;t-t_1)\chi(\mathbf{q}_1)K_0(\mathbf{q}_1-\mathbf{q}';t_1)\,. \tag{32}$$

Here, an important remark is in order. The energy-domain formulation of Kirchhoff diffraction, Eq. (30), only assumes the validity of the Helmholtz equation for a field in question, and is therefore applicable to a wide range of wave phenomena encountered, for instance, in acoustics, optics, and non-relativistic quantum mechanics. Equation (32) however relies on the particular relation, given by Eq. (5), between the energy-dependent Green function and time-dependent propagator, and is restricted to non-relativistic quantum mechanics only.

Also, we note that the physical picture implied by Eq. (32) is that of a particle traveling freely from $\mathbf{q}'$ to a point $\mathbf{q}_1$ in the aperture, and then from $\mathbf{q}_1$ to $\mathbf{q}$. It is therefore implicitly assumed that the aperture and points $\mathbf{q}$ and $\mathbf{q}'$ are chosen in such a way that every path $\mathbf{q}'\to\mathbf{q}_1\to\mathbf{q}'$ has no intersection with the screen other than at $\mathbf{q}_1$. In other words, Eq. (32) is only applicable to configurations in which apertures are not "shadowed" by S and are directly "visible" from the points $\mathbf{q}$ and $\mathbf{q}'$.

D. Diffraction in space and time

We now note a striking similarity between (i) the Huygens-Fresnel expansion of the propagator for the problem of diffraction in time, Eq. (18), and (ii) the time-dependent formulation of Kirchhoff theory, Eq. (32). This leads us to a conjecture that both expressions are particular cases of a more general propagator expansion, describing quantum diffraction on apertures which themselves may vary in the course of time. Such time-dependent apertures are represented by a characteristic function χ that depends on both the position $\mathbf{q}_1$ along the dividing surface S and the instant t_1 of the time interval $(0,t)$. As before, $\chi=\chi(\mathbf{q}_1;t_1)$ is allowed to take values between 0 (perfect absorption) and 1 (perfect transmission). In this case, we conjecture that the propagator, connecting two points $\mathbf{q}$ and $\mathbf{q}'$ on the opposite sides of the screen (such that $s(\mathbf{q}')<0$ and $s(\mathbf{q})>0$) in time t, is given by

$$K(\mathbf{q},\mathbf{q}';t) = \frac{1}{2}\int_0^t \mathrm{d}t_1\int_{\mathbb{R}^f}\mathrm{d}^f\mathbf{q}_1\,\delta\big(s(\mathbf{q}_1)\big) \\ \times\left(\frac{\mathbf{q}-\mathbf{q}_1}{t-t_1}+\frac{\mathbf{q}_1-\mathbf{q}'}{t_1}\right)\cdot\boldsymbol{\nabla}s(\mathbf{q}_1) \\ \times K_0(\mathbf{q}-\mathbf{q}_1;t-t_1)\chi(\mathbf{q}_1;t_1)K_0(\mathbf{q}_1-\mathbf{q}';t_1)\,. \tag{33}$$

Equation (33), which from now on we will refer as to Huygens-Fresnel-Kirchhoff (HFK) construction, constitutes the main result of the present paper.

Our arguments supporting the conjecture, given by Eq. (33), are as follows. First, the propagator expansion is in accord with the Huygens-Fresnel principle. Second, the HFK construction correctly captures the physics of diffraction in time: In the special case that χ is independent of $\mathbf{q}_1$ and that the surface S is given by an $(f-1)$-dimensional plane, $s(\mathbf{q}_1)=\mathbf{n}\cdot(\mathbf{q}_1-\mathbf{q}_0)$ with a unit vector $\mathbf{n}$ and some fixed vector $\mathbf{q}_0$, Eq. (33) becomes equivalent to Eq. (18) with x, x', and x_1 replaced, respectively, by $\mathbf{n}\cdot\mathbf{q}$, $\mathbf{n}\cdot\mathbf{q}'$, and $\mathbf{n}\cdot\mathbf{q}_1$. Third, in the case that χ is independent of t_1, Eq. (33) is nothing but a time-dependent formulation of Kirchhoff diffraction.

III. DIFFRACTION OF SPATIALLY LOCALIZED WAVE PACKETS

In this section, we apply the HFK construction, Eq. (33), to wave functions that are initially localized in position space. We direct out attention to some example systems in one and two spatial dimensions.

As before, we consider an absorbing screen that is defined by a surface S, Eq. (29), and a characteristic function χ. The latter, in general, is a function both of the position on S and of time. We further consider a quantum particle described at time $t=0$ by a wave function $\Psi(\mathbf{q}';0)$, which is localized in a small neighborhood of a linear size σ around a spatial point $\mathbf{Q}$, i.e., $\Psi(\mathbf{q}';0)\simeq 0$ for $|\mathbf{q}'-\mathbf{Q}|\gg\sigma$. Here, we consider the case of σ being small compared to the distance L between the point $\mathbf{Q}$ and the surface S. For concreteness, we take $s(\mathbf{Q})<0$. Then, in accordance with Eqs. (1) and (33), the wave function Ψ at a point $\mathbf{q}$, such that $s(\mathbf{q})>0$, and time $t>0$ can be approximately written as

$$\Psi(\mathbf{q};t) \simeq \frac{1}{2}\int_0^t \mathrm{d}t_1\int_{\mathbb{R}^f}\mathrm{d}^f\mathbf{q}_1\,\delta\big(s(\mathbf{q}_1)\big) \\ \times\left(\frac{\mathbf{q}-\mathbf{q}_1}{t-t_1}+\frac{\mathbf{q}_1-\mathbf{Q}}{t_1}\right)\cdot\boldsymbol{\nabla}s(\mathbf{q}_1) \\ \times K_0(\mathbf{q}-\mathbf{q}_1;t-t_1)\chi(\mathbf{q}_1;t_1)\Psi_0(\mathbf{q}_1;t_1)\,, \tag{34}$$

where

$$\Psi_0(\mathbf{q}_1;t_1) = \int_{\mathbb{R}^f}\mathrm{d}^f\mathbf{q}'\,K_0(\mathbf{q}_1-\mathbf{q}';t_1)\Psi(\mathbf{q}';0) \tag{35}$$

is the wave function of the corresponding free particle. Equation (34) holds to the leading order in the small parameter σ/L.

A. One dimension

As our first example we consider the Moshinksy problem in one dimension ($f = 1$) for a quantum particles initially described by the Gaussian wave packet

$$\Psi(x';0) = \left(\frac{1}{\pi\sigma^2}\right)^{\frac{1}{4}} \exp\left(\frac{i}{\hbar}P(x'-Q) - \frac{(x'-Q)^2}{2\sigma^2}\right). \tag{36}$$

Here, Q and P represent, respectively, the average position and momentum of the particle, and σ characterizes the wave packet dispersion in the position space. In our set-up, an absorbing shutter is placed at a point d, such that $Q < d$ and $\sigma \ll L = d - Q$. We are interested in the wave function $\Psi(x;t)$ at $x > d$ and $t > 0$.

A substitution of Eq. (36), along with $s(x_1) = x_1 - d$ and $\chi = \chi(t_1)$, into Eqs. (34) and (35) yields

$$\Psi(x;t) \simeq \frac{1}{2}\int_0^t \mathrm{d}t_1 \left(\frac{x-d}{t-t_1} + \frac{d-Q}{t_1}\right) \times K_0(x-d;t-t_1)\chi(t_1)\Psi_0(d;t_1) \tag{37}$$

with

$$\Psi_0(x;t) = \left(\frac{1}{\pi\gamma_t^2\sigma^2}\right)^{\frac{1}{4}} \times \exp\left(\frac{i}{\hbar}\frac{P^2}{2m}t + \frac{i}{\hbar}P(x-Q_t) - \frac{(x-Q_t)^2}{2\gamma_t\sigma^2}\right) \tag{38}$$

and

$$Q_t = Q + \frac{P}{m}t \quad \text{and} \quad \gamma_t = 1 + i\frac{\hbar t}{m\sigma^2}. \tag{39}$$

Evaluating the integral in the right-hand side of Eq. (37) numerically on obtains the wave function $\Psi(x,t)$ at $x > d$ and $t > 0$.

Figure 1 shows the diffraction patterns calculated in accordance with Eq. (37) for different shutter protocols, $\chi(t_1)$. The initial wave packet, Eq. (36), is centered around $Q = 0$ and has the average momentum $P = 200$ and the position dispersion $\sigma = 0.1$. Hereinafter, we use the atomic units, $m = \hbar = 1$, in all numerical examples. The absorbing shutter is positioned at $d = 8$. Figure 1 shows the probability density $|\Psi(x,t)|^2$ as a function of x for a fixed time, $t = 0.05$. Note that, for our choice of parameters, the position at the time t of the corresponding free classical particle is $Q_t = Q + Pt/m = 10$. The figure shows four probability density distributions for (i) $\chi(t_1) = 1$, representing the free-particle case, (ii) $\chi(t_1) = \Theta(t_1 - t_0)$, corresponding to the perfectly absorbing shutter first being in place and then suddenly removed at time t_0, (iii) $\chi(t_1) = \Theta(t_0 - t_1)$, corresponding to the shutter closed instantaneously at t_0, and (iv) $\chi(t_1) = \Theta(1 - |t_1 - t_0|/\epsilon)$, representing a scenario in which the shutter is open only during a time interval of half-width ϵ centered around t_0. Here we take $t_0 = 0.04$ and $\epsilon = 5 \times 10^{-4}$. Note that the position at time t_0 of the corresponding free classical particle is $Q + Pt_0/m = 8$ and coincides with the position of the shutter.

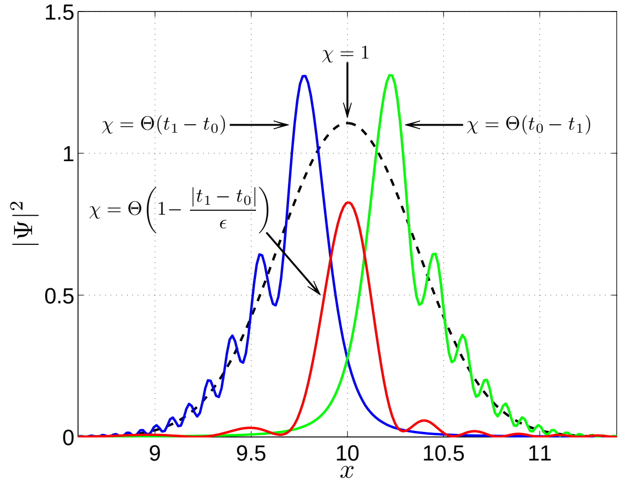

FIG. 1: (Color online) The probability density $|\Psi(x,t)|^2$, calculated in accordance with Eq. (37) for various characteristic functions $\chi(t_1)$, as a function of the position x. The initial wave packet is characterized by its position $Q = 0$, average momentum $P = 200$, and dispersion $\sigma = 0.1$. The position of the shutter is given by $d = 8$, and the propagation time is $t = 0.05$. The shutter switching time $t_0 = 0.04$ and the time window $\epsilon = 5 \times 10^{-4}$. All quantities are given in the atomic units, $m = \hbar = 1$.

Oscillations in the spatial dependence of the probability density, seen distinctly in Fig. 1, are introduced by an instantaneous process of switching the shutter, and are, in fact, a manifestation of the diffraction-in-time phenomenon. It is well known that these oscillations become less pronounced and eventually disappear as one switches the shutter "continuously" over longer and longer time intervals [10, 18]. Here we note that the HFK construction provides a convenient framework for analyzing the disappearance (also known as apodization) of the diffraction pattern for initial states that are localized in the position space. The phenomenon of the apodization of atomic beams, which correspond to initial states localized in the momentum space, has been previously addressed by different methods [17, 18].

B. Two dimensions

We now address diffraction of quantum wave packets in two dimensions on a (generally curved) shutter whose absorption properties may both depend on position and vary in time. We consider a quantum particle with the initial state given by

$$\Psi(x,y;0) = \phi_1(x,0)\,\phi_2(y,0), \tag{40}$$

where

$$\phi_j(\zeta,0) = \left(\frac{1}{\pi\sigma_j^2}\right)^{\frac{1}{4}} \exp\left(\frac{i}{\hbar}P_j(\zeta-Q_j) - \frac{(\zeta-Q_j)^2}{2\sigma_j^2}\right) \tag{41}$$

for $j=1$ and 2. Here, $\mathbf{Q}=(Q_1,Q_2)$ is the average position and $\mathbf{P}=(P_1,P_2)$ average momentum of the particle, and σ_1 and σ_2 characterize respectively the x- and y-component of the wave packet dispersion in the position space. As in the one-dimensional case, the initial distance between the particle and the shutter is assumed to be large compared to the spatial extent of the wave packet.

Analogously to Eqs. (38) and (39), the time evolution of a free particle is described by the wave function

$$\Psi_0(x,y;t) = \phi_1(x,t)\,\phi_2(y,t)\,, \tag{42}$$

where

$$\phi_j(\zeta,t) = \left(\frac{1}{\pi\gamma_{j,t}^2\sigma_j^2}\right)^{\frac{1}{4}} \exp\left[\frac{i}{\hbar}\frac{P_j^2}{2m}t + \frac{i}{\hbar}P_j(\zeta-Q_{j,t}) - \frac{(\zeta-Q_{j,t})^2}{2\gamma_{j,t}\sigma_j^2}\right] \tag{43}$$

and

$$Q_{j,t} = Q_j + \frac{P_j}{m}t \quad \text{and} \quad \gamma_{j,t} = 1 + i\frac{\hbar t}{m\sigma_j^2}\,, \tag{44}$$

for $j=1$ and 2. Then, using this expression for Ψ_0 in Eq. (34) and evaluating numerically the two-dimensional integral (over time and along a one-dimensional curve accommodating the shutter), we obtain the wave function $\Psi(x,y;t)$ at $t>0$ and at a point (x,y) on the side of the shutter opposite to $\mathbf{Q}$.

Figure 2 illustrates the effect of shutter curvature on the diffraction pattern. The set-up is schematically presented in Fig. 2a. The initial state of the particle is given by a Gaussian wave packet, Eqs. (40) and (41), with the average position $\mathbf{Q}=(0,0)$, average momentum $\mathbf{P}=(200,0)$, and dispersion $\sigma_1=\sigma_2=0.1$. The wave packet is incident upon a shutter, whose spatial geometry is defined by the curve $s(x_1,y_1)=x_1-d-\alpha y_1^2=0$ with $d=8$. Depending on the sign of the parameter α, the shutter is concave ($\alpha<0$), flat ($\alpha=0$), or convex ($\alpha>0$). The time dependence of the shutter is given by the characteristic function $\chi(\mathbf{q}_1;t_1)=\Theta(1-|t_1-t_0|/\epsilon)$ with $t_0=0.04$ and $\epsilon=5\times10^{-4}$. This corresponds to the case of a perfectly absorbing shutter that is open only during a time interval of half-width ϵ centered around t_0 (cf. solid red curve in Fig. 1). The propagation time is set to $t=0.05$, and the wave function is investigated inside a spatial region defined by $8.9<x<11.1$ and $-1.6<y<1.6$, shown schematically as a (light blue) rectangle in Fig. 2a. Note that the position of the corresponding classical particle at time t equals $\mathbf{Q}_t=\mathbf{Q}+\mathbf{P}t/m=(10,0)$ and coincides with the center of the rectangle. Then, the logarithm of the probability density, $\ln|\Psi(x,y;t)|^2$, inside the rectangular region is shown for three different values of the parameter α: Fig. 2b corresponds to $\alpha=-0.3$ (concave shutter), Fig. 2c to $\alpha=0$ (flat shutter), and Fig. 2d to $\alpha=0.3$ (convex shutter). While the mean position of the quantum particle coincides with that of the corresponding classical particle, the diffraction patterns are clearly different for the three choices of α. Compared to the diffraction pattern produced by the flat shutter, the concave shutter gives rise to a "divergent" pattern, while the convex shutter produces a "convergent" diffraction pattern.

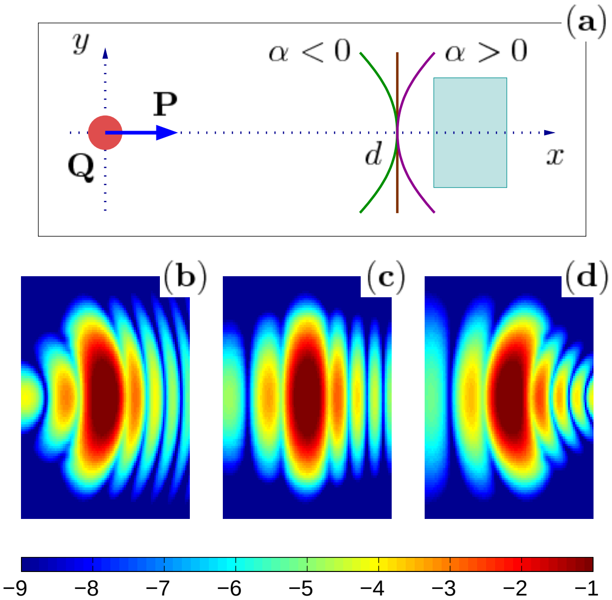

FIG. 2: (Color online) Diffraction in time on a curved shutter. Part (a) of the figure illustrates the set-up. The initial wave packet is characterized by its average position $\mathbf{Q}=(0,0)$, average momentum $\mathbf{P}=(200,0)$, and dispersion $\sigma_1=\sigma_2=0.1$. The shutter is positioned along the curve $s(x_1,y_1)=x_1-d-\alpha y_1^2=0$ with $d=8$, and its time dependence is specified by $\chi(t_1)=\Theta(1-|t_1-t_0|/\epsilon)$ with $t_0=0.04$ and $\epsilon=5\times10^{-4}$. The propagation time is $t=0.05$. The (light blue) rectangle, covering $8.9<x<11.1$ and $-1.6<y<1.6$, outlines the spatial region, in which the probability density is computed. Parts (b), (c), and (d) of the figure show $\ln|\Psi(x,y;t)|^2$ for $\alpha=-0.3$, 0, and 0.3 respectively. All quantities are given in the atomic units, $m=\hbar=1$.

Figure 3 addresses diffraction on a flat screen whose absorbing properties depend on time as well as vary in space. The set-up, schematically illustrated in Fig. 3a. As before, the initial wave packet is described by $\mathbf{Q}=(0,0)$, $\mathbf{P}=(200,0)$, $\sigma_1=\sigma_2=0.1$, and the propagation time is $t=0.05$. Here we consider a flat screen, given by $s(x_1,y_1)=x_1-d$ with $d=8$, and study diffraction patterns for three different characteristic functions χ. As in Fig. 2, we present the logarithm of the probability density, $\ln|\Psi(x,y;t)|^2$, inside a spatial region defined by $8.9<x<11.1$ and $-1.6<y<1.6$, and illus-

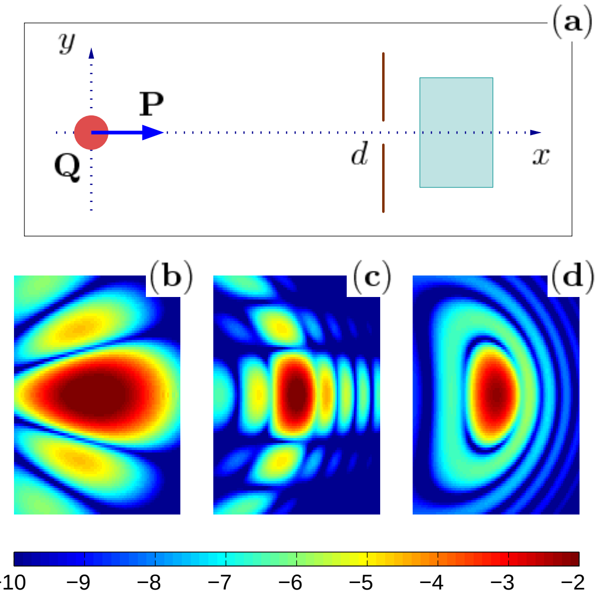

FIG. 3: (Color online) Diffraction on a flat absorbing screen with a time-dependent aperture. Part (a) of the figure illustrates the set-up. Parameters of the initial wave packet are the same as in Fig. 2: $\mathbf{Q} = (0, 0)$, $\mathbf{P} = (200, 0)$, and $\sigma_1 = \sigma_2 = 0.1$. The propagation time is $t = 0.05$. The plane of the absorbing screen is defined by $s(x_1, y_1) = x_1 - d$ with $d = 8$. The (light blue) rectangle, covering $8.9 < x < 11.1$ and $-1.6 < y < 1.6$, outlines the spatial region, in which the probability density is computed. Parts (b), (c), and (d) of the figure show $\ln |\Psi(x, y; t)|^2$ for $\chi(\mathbf{q}_1; t_1)$ equal, respectively, to $\Theta(1 - |y_1|/\delta)$, $\Theta(1 - |y_1|/\delta)\Theta(1 - |t_1 - t_0|/\epsilon)$, and $\big(1 - y_1^2/\delta^2 - (t_1 - t_0)^2/\epsilon^2\big)$ with $\delta = 0.05$, $t_0 = 0.04$, and $\epsilon = 5 \times 10^{-4}$. All quantities are given in the atomic units, $m = \hbar = 1$.

trated by a (light blue) rectangle. Figure 3b shows the diffraction pattern produced by a slit in the absorbing screen and corresponds to $\chi(\mathbf{q}_1; t_1) = \Theta(1 - |y_1|/\delta)$ with $\delta = 0.05$. Figure 3c represents a scenario, in which the slit of spatial half-width δ is open only during a time interval of half-width $\epsilon = 5 \times 10^{-4}$ centered around time $t_0 = 0.04$. The corresponding characteristic function is $\chi(\mathbf{q}_1; t_1) = \Theta(1 - |y_1|/\delta)\Theta(1 - |t_1 - t_0|/\epsilon)$. Figure 3d shows the diffraction pattern obtained for the characteristic function $\chi(\mathbf{q}_1; t_1) = \Theta\big(1 - y_1^2/\delta^2 - (t_1 - t_0)^2/\epsilon^2\big)$. In this case, the width of the slit continuously increases from 0 to 2δ during the time interval $t_0 - \epsilon < t_1 < t_0$, and then shrinks back to 0 during $t_0 < t_1 < t_0 + \epsilon$.

It is interesting to observe some similarity of, on one hand, the diffraction patterns of Figs. 3c and 3d, and, on the other hand, patterns of Fraunhofer diffraction of light on, respectively, rectangular and elliptic apertures in opaque two-dimensional screens (e.g., see Figs. 8.10 and 8.12 in Ref. [6]). The similarity becomes even stronger when one takes into account the space-time, (y_1, t_1) representation of the apertures leading to the diffraction patterns shown in Figs. 3c and 3d. Indeed, the aperture defined by the characteristic function $\chi(\mathbf{q}_1; t_1) = \Theta(1 - |y_1|/\delta)\Theta(1 - |t_1 - t_0|/\epsilon)$ can be represented as a rectangular opening in the (y_1, t_1) coordinates, while the aperture corresponding to $\chi(\mathbf{q}_1; t_1) = \Theta\big(1 - y_1^2/\delta^2 - (t_1 - t_0)^2/\epsilon^2\big)$ has the shape of an ellipse in the same coordinates. This observation suggests that f-dimensional quantum dynamics in the presence of time-dependent diffracting obstacles may be used for modeling diffraction in $(f + 1)$-dimensional systems with stationary, time-independent obstacles.

IV. CONCLUSIONS

In this paper we have revisited the phenomenon of diffraction in non-relativistic quantum mechanics. More specifically, we have considered the problem of a quantum particle passing through an opening (or a set of openings) in a perfectly absorbing screen. Having assumed the validity of the Huygens-Fresnel principle, we have constructed an expansion of the quantum propagator that connects two spatial points lying on the opposite sides of the screen. The expansion represents the full propagator as a sum of products of two free particle propagators, one connecting the initial point and the other connecting the final point to a point in the opening. The construction holds in the cases of curved (convex or concave) screens and for openings whose shape changes in time. Consequently, our approach allows one to analyze the quantum phenomena of diffraction in space and diffraction in time, as well as the interplay between the two.

In order to illustrate the method, we have used our propagator expansion to calculate diffraction patterns for an initially localized wave packet passing through various spatio-temporal diffraction screens in one and two dimensions. Thus, in two dimensions, we have investigated the effect of screen curvature on the diffraction pattern by analyzing diffraction in time produced by absorbing parabolic shutters and demonstrating how a convex (concave) shutter gives rise to effective focusing (defocusing) of the wave function. We have also studied diffraction of spatially localized wave packets passing through holes of time-dependent size. We have shown that the shape of a diffracted wave function is largely determined by the space-time geometry of the hole, suggesting the use of time-dependent obstacles in f-dimensional systems for modeling quantum diffraction on stationary obstacles in $(f + 1)$-dimensional systems.

The approach, developed in this paper, is applicable to quantum diffraction on perfectly absorbing screens, and, therefore, complements the method of Brukner and Zeilinger [15] valid for perfectly reflecting screens. In laboratory experiments, however, diffraction screens are typically neither perfectly absorbing nor perfectly reflecting, and the two methods have to be used in combination. It would interesting to develop such a unified approach and to test its predictions against results of experimental measurements.

Acknowledgments

The author would like to thank Joshua Bodyfelt, Andre Eckardt, Orestis Georgiou, Klaus Hornberger, Roland Ketzmerick, Klaus Richter, Roman Schubert, Akira Shudo, Martin Sieber, and Steven Tomsovic for helpful discussions and comments at various stages of this project.

Appendix A: Derivation of Eqs. (10) and (11)

In one dimension the free-particle Green function, $G_0(l;E)$ with $l>0$, is given by

$$\begin{aligned} G_0(l;E) &= \mathcal{L}[K_0](l;s) = \int_0^\infty \mathrm{d}t\, \mathrm{e}^{-st} K_0(l;t) \\ &= \sqrt{\frac{m}{2\pi i\hbar}} \int_0^\infty \frac{\mathrm{d}t}{\sqrt{t}} \exp\left(-\frac{ml^2}{2i\hbar t} - st\right) \\ &= \sqrt{\frac{m}{2i\hbar s}} \exp\left(-l\sqrt{\frac{2ms}{i\hbar}}\right). \end{aligned} \tag{A1}$$

Here, $s = E/(i\hbar)$ is implied, cf. Eq. (5), and the reader is referred to the formula 3.471.15 of Ref. [24] for the last integral.

We now consider the integral

$$\mathcal{I} \equiv \int_0^t \mathrm{d}t_1\, K_0(x-x_1;t-t_1) K_0(x_1-x';t_1)\,, \tag{A2}$$

where x, x', and x_1 satisfy Eq. (7). The Laplace transform of $\mathcal{I}$ is given by

$$\begin{aligned} \mathcal{L}[\mathcal{I}] &= \mathcal{L}[K_0](x-x_1;s)\, \mathcal{L}[K_0](x_1-x';s) \\ &= \frac{m}{2i\hbar s} \exp\left(-(x-x')\sqrt{\frac{2ms}{i\hbar}}\right) \\ &= \sqrt{\frac{m}{2i\hbar s}}\, \mathcal{L}[K_0](x-x';s)\,. \end{aligned} \tag{A3}$$

Then, using the fact that $1/\sqrt{s} = \mathcal{L}[1/\sqrt{\pi t}]$ and performing the inverse Laplace transform, we obtain

$$\begin{aligned} \mathcal{I} &= \sqrt{\frac{m}{2\pi i\hbar}} \int_0^t \frac{\mathrm{d}t_1}{\sqrt{t-t_1}} K_0(x-x';t_1) \\ &= \frac{m}{2\pi i\hbar} \int_0^t \frac{\mathrm{d}t_1}{\sqrt{t_1(t-t_1)}} \exp\left(-\frac{m(x-x')^2}{2i\hbar t_1}\right). \end{aligned} \tag{A4}$$

The integral in the last line of Eq. (A4) is given by the formula 3.471.2 of Ref. [24],

$$\begin{aligned} &\int_0^t \frac{\mathrm{d}t_1}{\sqrt{t_1(t-t_1)}} \exp\left(-\frac{\beta}{t_1}\right) \\ &\quad = \sqrt{\pi}\left(\frac{t}{\beta}\right)^{\frac{1}{4}} \exp\left(-\frac{\beta}{2t}\right) W_{-\frac{1}{4},\frac{1}{4}}\left(\frac{\beta}{t}\right), \end{aligned} \tag{A5}$$

where W stands for the Whittaker function. The latter can be written as (see page 341 in Ref. [25], or section 13.18(ii) of Ref. [26])

$$W_{-\frac{1}{4},\frac{1}{4}}(\zeta^2) = \sqrt{\pi z}\, \exp(\zeta^2/2)\, \mathrm{erfc}(\zeta) \tag{A6}$$

with "erfc" denoting the complementary error function.

Substituting Eqs. (A5) and (A6) into (A4) we obtain

$$\mathcal{I} = \frac{m}{2i\hbar}\, \mathrm{erfc}\left(\sqrt{\frac{m}{2i\hbar t}}(x-x')\right). \tag{A7}$$

A comparison of the right-hand sides of Eqs. (A2) and (A7) completes the proof of the identity (9) with the function u chosen in accordance with Eq. (11).

In order to prove that Eq. (10) offers an alternative choice for the function u we consider

$$\mathcal{I}' \equiv \left(\eta_1 \frac{\partial}{\partial x} + \eta_2 \frac{\partial}{\partial x'}\right)\mathcal{I}\,, \tag{A8}$$

where $\mathcal{I}$ is given by Eq. (A2), and η_1 and η_2 are two arbitrary, generally complex numbers. On one hand, $\mathcal{I}'$ can be evaluated by a direct substitution of Eq. (A2) into Eq. (A8) which leads to

$$\begin{aligned} \mathcal{I}' = \frac{im}{\hbar} \int_0^t \mathrm{d}t_1 &\left(\eta_1 \frac{x-x_1}{t-t_1} - \eta_2 \frac{x_1-x'}{t_1}\right) \\ &\times K_0(x-x_1;t-t_1) K_0(x_1-x';t_1)\,. \end{aligned} \tag{A9}$$

On the other hand, using Eqs. (A8), (A3), and (A1), we have

$$\begin{aligned} \mathcal{L}[\mathcal{I}'] &= \left(\eta_1 \frac{\partial}{\partial x} + \eta_2 \frac{\partial}{\partial x'}\right) \mathcal{L}[\mathcal{I}](x-x';s) \\ &= \sqrt{\frac{m}{2i\hbar s}} \left(\eta_1 \frac{\partial}{\partial x} + \eta_2 \frac{\partial}{\partial x'}\right) \mathcal{L}[K_0](x-x';s) \\ &= \frac{im}{\hbar}(\eta_1-\eta_2)\mathcal{L}[K_0](x-x';s)\,, \end{aligned} \tag{A10}$$

and therefore

$$\mathcal{I}' = \frac{im}{\hbar}(\eta_1-\eta_2) K_0(x-x';t)\,. \tag{A11}$$

Finally, comparing Eqs. (A9) and (A11), and introducing a complex number $\eta = \eta_1/(\eta_1-\eta_2)$, we arrive at the identity (9) with the function u given by Eq. (10).

[1] A. D. Cronin, J. Schmiedmayer, and D. E. Pritchard, Rev. Mod. Phys. **81**, 1051 (2009).

[2] M. Arndt, O. Nairz, J. Vos-Andreae, C. Keller, G. van der Zouw, and A. Zeilinger, Nature **401**, 680 (1999).

[3] B. Brezger, L. Hackermüller, S. Uttenthaler, J. Petschinka, M. Arndt, and A. Zeilinger, Phys. Rev. Lett. **88**, 100404 (2002).

[4] L. Hackermüller, S. Uttenthaler, K. Hornberger, E. Reiger, B. Brezger, A. Zeilinger, and M. Arndt, Phys. Rev. Lett. **91**, 090408 (2003).

[5] B. B. Baker and E. T. Copson, *The mathematical theory of Huygen's principle* (Clarendon Press, Oxford, 1950), 2nd ed.

[6] M. Born and E. Wolf, *Principles of optics* (Cambridge University Press, 1999), 7th ed.

[7] M. Moshinsky, Phys. Rev. **88**, 625 (1952).

[8] P. Szriftgiser, D. Guéry-Odelin, M. Arndt, and J. Dalibard, Phys. Rev. Lett. **77**, 4 (1996).

[9] M. Kleber, Phys. Rep. **236**, 331 (1994).

[10] A. del Campo, G. García-Calderón, and J. G. Muga, Phys. Rep. **476**, 1 (2009).

[11] R. P. Feynman and A. R. Hibbs, *Quantum Mechanics and Path Integrals* (McGraw-Hill, New York, 1965).

[12] A. Zecca, Int. J. Theor. Phys. **38**, 911 (1999).

[13] M. Gondran and A. Gondran, Am. J. Phys. **73**, 507 (2005).

[14] G. Glionna, A. H. Blin, B. Hiller, M. C. Nemes, M. Sampaio, and A. F. R. de Toledo Piza, Physica A **387**, 1485 (2008).

[15] C. Brukner and A. Zeilinger, Phys. Rev. A **56**, 3804 (1997).

[16] G. Kälbermann, J. Phys. A: Math. Gen. **35**, 4599 (2002).

[17] A. del Campo and J. G. Muga, J. Phys. A: Math. Gen. **38**, 9803 (2005).

[18] A. del Campo, J. G. Muga, and M. Moshinsky, J. Phys. B: At. Mol. Opt. Phys. **40**, 975 (2007).

[19] L. S. Schulman, *Techniques and Applications of Path Integration* (Wiley, New York, 1981).

[20] J. G. Muga, J. P. Palao, B. Navarro, and I. L. Egusquiza, Phys. Rep. **395**, 357 (2004).

[21] J. F. Nye, J. H. Hannay, and W. Liang, Proc. R. Soc. Lond. A **449**, 515 (1995).

[22] J. H. Hannay, Proc. R. Soc. Lond. A **450**, 51 (1995).

[23] J. H. Hannay, Phil. Trans. R. Soc. Lond. A **359**, 1473 (2001).

[24] I. S. Gradshteyn and I. M. Ryzhik, *Table of integrals, series, and products* (Elsevier/Academic Press, Amsterdam, 2007), 7th ed.

[25] E. T. Whittaker and G. N. Watson, *A Course of Modern Analysis* (Cambridge University Press, 1927), 4th ed.

[26] *Digital Library of Mathematical Functions* (National Institute of Standards and Technology, 2010), URL `http://dlmf.nist.gov/`.