Survival probability of a quantum particle in the presence of an absorbing surface

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We propose a formulation of an absorbing boundary for a quantum particle. The formulation is based on a Feynman-type integral over trajectories that are confined by an absorbing boundary. Trajectories that reach the absorbing wall are instantaneously terminated and their probability is discounted from the population of the surviving trajectories. This gives rise to a unidirectional absorption current at the boundary. We calculate the survival probability as a function of time. Several applications are given: the calculation of the absorption current in the slit experiment with a totally absorbing screen, the calculation of the survival probability of a particle between two totally absorbing walls, and the calculation of the survival probability and of the reflection coefficient of a Gaussian wave packet incident on a totally absorbing wall. The survival probability of a one-dimensional particle between two totally absorbing walls exhibits decay with beats.

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I. INTRODUCTION

A standard scattering experiment with absorption consists of firing electrons at a scintillation screen or a photographic plate and recording the times and places where they are absorbed in the target. In an ideal situation, once observed in the target the particle never leaves it. The histograms of times and places of absorption are recorded, including electrons that are not absorbed (e.g., electrons that are reflected, transmitted, or never reach the target). The histogram gives also the survival probability of a particle outside the target, denoted $S(t)$, which is the probability of the particle not being absorbed by time t. The survival probability $S(t)$ decreases in time, indicating that a net probability current flows into the target. If the absorber is ideal the flow is unidirectional into the target [1].

The description of this experiment in terms of a wave function of a particle is expected to start with a wave function that is localized outside the target and in time breaks into two parts, $\psi(x,t)=\psi_1(x,t)+\psi_2(x,t)$, such that

$$S(t)=\int_{D^c}|\psi_1(x,t)|^2\,dx,$$

where the domain D^c is the space outside the target, and $\psi_1(x,t)$ is orthogonal to $\psi_2(x,t)$ at time t. For all times $s>t$ the functions $\psi_1(x,s)$ and $\psi_2(x,s)$ evolve independently of each other. The wave function $\psi(x,t)$ is expected to separate into two such components at least in the case of ideal absorption (this may be called a ‘‘separation principle’’ of wave functions). In each time interval $[t,t+\Delta t]$ the survival probability of the particle has to be discounted by the absorption probability in this time interval [see Eq. (4.9)]. Such ideal absorption may be due to internal processes within the target.

No such separation, however, exists in quantum theory of scattering on a real-valued potential localized in a bounded domain D. More precisely, there is no known real-valued Hamiltonian that reproduces the above partition of the wave function. A complex-valued potential has been devised in [2–5] to produce total absorption of an incident wave on a target. More specifically, for each mode e^{ikx} a complex potential of arbitrarily small width can be constructed so that the reflection and transmission coefficients for this mode vanish. This is interpreted as total absorption of this mode in the potential. A series of such potentials absorbs a discrete set of modes. In this paper, we propose a formalism for the construction of the survival probability $S(t)$ of a quantum particle in the presence of an ideal absorbing wall and for the construction of the conditional wave function of the particle, given that it has not been absorbed by time t.

We adopt an approach to absorption based on the Feynman integral, analogous to the approach to absorption used in the Wiener integral. Our approach is based on the definition of an ideal absorber as a wall that absorbs all Feynman trajectories that reach it. Their absorption is total in the sense that every Feynman trajectory that reaches the absorber is terminated there and then instantaneously is totally absorbed. The survival probability at time t is the probability of all Feynman trajectories that have not reached the absorbing wall by time t. In the proposed theory some of the requirements of a model of absorption are satisfied, namely, the wave function is separated into two noninterfering parts and the survival probability of the unabsorbed part is calculated. The evolution of the particle after absorption is not discussed here.

Rather than developing a definition of ideal absorbers from a Hamiltonian formulation with many degrees of freedom, as done, for example, in [6] and which leads to complex potentials, we adopt an axiomatic approach that at-

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tempts to capture the essence of the mathematical phenomenology involved in quantum absorption processes that are experimentally observed. In this definition nothing is said about the underlying mechanism that causes absorption so that the more basic question of how absorption comes about is not answered in the proposed theory. This definition may be a fundamental notion in quantum mechanics or it may possibly be derived from existing tenets of quantum mechanics.

We find from our formalism that the conditional wave function to be at a given point at a given time, given that the particle survived so far, satisfies Schrödinger's equation with reflecting boundary conditions on the absorbing surface and we calculate the survival probability $S(t)$. Since the wave function of the unabsorbed particle vanishes beyond the absorbing wall, it suffers a discontinuity in its derivative across the absorbing surface [7–9]. Clearly, the wave function of the particle to survive and be at x at time t is not the same as the conditional wave function, given that the particle has not been absorbed by time t. The former is normalized to $S(t)$ whereas the latter is normalized to 1.

In Sec. II we formulate the postulates of absorption in a surface and explain the discounting procedure. In Sec. III we calculate the Feynman integral over the class of trajectories that are bounded within a given boundary and show that it satisfies Schrödinger's equation with total reflection on the boundary. In Sec. IV we calculate the probability of Feynman trajectories that propagate into the absorbing boundary and obtain the survival probability of the unabsorbed trajectories. In Sec. V we calculate the absorption current at the absorbing boundary and consider the slit experiment with an absorbing screen. Section VI contains two examples: a one-dimensional particle between totally absorbing walls and a Gaussian wave packet incident on a totally absorbing wall. Finally, a discussion and summary are offered in Sec. VII.

II. THE POSTULATES OF ABSORPTION IN A SURFACE

The two simplest types of instantaneous absorption at a wall are the absorption of all Feynman trajectories when they reach the wall for the first time, or the absorption of trajectories that propagate across the wall. It was shown in [7–12] that Feynman integrals over the set of trajectories that terminate at a given wall produce wave functions that vanish on and beyond the wall. The resulting wave functions are continuous, though they have discontinuous derivatives on the boundaries of their supports. It was shown in [1] that for this type of initial wave function the probability that propagates across the boundary of the support in a short time Δt is proportional to $\Delta t^{3/2}$ so that a continuous discounting of the wave function by the probability of the trajectories that crossed into the absorbing domain beyond the wall leads to total reflection, much like in the Zeno effect [13]. It is shown below that the probability density that propagates into an absorbing wall in a short time Δt is proportional to Δt, so that discounting the probability of these trajectories leads to a decay law, consequently, we adopt the concept of instantaneous absorption at a wall for wave functions that vanish on and beyond the wall. More specifically, in our Feynman-type integral trajectories that propagate into the surface for the first time are considered to be absorbed instantaneously or reflected with a given probability which is a property of the interaction between the particle and the absorbing surface. The absorbed trajectories are therefore terminated at that surface. The probability of the absorbed trajectories at each time step is discounted from the population of the surviving trajectories. The instantaneous absorption rate is assumed proportional to the number (probability) of particles at the absorbing surface at a given moment of time. The proportionality constant is a characteristic length λ, determined by the absorbing material, e.g., photographic plate or scintillation screen, and by the absorbed particle, e.g., electron or neutron. In this paper λ is assumed constant. Under this assumption λ can be determined experimentally by measuring the absorption rate of a single energy level and then the measured λ can be used to calculate the absorption rate of any other energy level, in some energy range, or the simultaneous absorption of several energy levels in this range. The constant λ can be assumed to contain a multiplicative factor that represents the probability of absorption of a trajectory when it hits the wall. It is not clear whether λ is a new fundamental constant or can be derived from existing theory. Therefore, in this respect, the proposed theory can be equally termed phenomenological or a genuine extension of quantum mechanics.

In general, if the trajectories are partitioned into two subsets, the part of the wave function obtained from the Feynman integral over one subset cannot be used to calculate the probability of this subset due to interference between the wave functions of the two subsets. However, in the physical situation under consideration, such a calculation may be justified as follows. Our procedure, in effect, assumes a partition of all the possible trajectories at any given time interval $[t,t+\Delta t]$ into two classes. One is a class of *bounded trajectories* that have not reached the absorbing surface by time $t+\Delta t$ and remain in the domain, and the other is a class of trajectories that arrived at the surface for the first time in the interval $[t,t+\Delta t]$. We assume that the part of the wave function obtained from the Feynman integral over trajectories that reached the surface in this time interval no longer interferes in a significant way with the part of the wave function obtained from the Feynman integral over the class of restricted trajectories. The interference is terminated at this point so that the general population of trajectories can be discounted by the probability of the terminated trajectories. This assumption makes it possible to calculate separately the probability of the absorbed trajectories in the time interval $[t,t+\Delta t]$. The assumptions discussed above can be summarized in the form of the following postulates.

(i) The absorption of Feynman trajectories represents absorption of actual trajectories of particles.

(ii) The population of Feynman trajectories can be discounted by the probability of the absorbed trajectories.

In the language of wave functions the postulates (i) and (ii) can be replaced by postulate (iii).

(iii) The survival probability decreases by the probability that propagates at the absorbing wall at each time step.

The Feynman path-integral formulation of the postulates gives an intuitively simple picture of absorption. This picture is similar to that of the analogous picture in the Wiener integral formulation of absorption in diffusion theory [14].

III. THE FEYNMAN INTEGRAL OVER BOUNDED TRAJECTORIES

If a quantum particle is constrained in space to a finite (or semifinite) domain, the Feynman integral has to be confined to Feynman trajectories that stay forever in this domain. This implies the following modification in the definition of the Feynman integral. The function space is now the class

$$\sigma_{a,b}=\{x(\cdot)\in C[0,t]|a\leqslant x(\tau)\leqslant b,0\leqslant \tau\leqslant t\}$$

and the definition of the Feynman integral over the class $\sigma_{a,b}$ is

$$K_{a,b}(x,t)=\int_{\sigma_{a,b}}\exp\left\{\frac{i}{\hbar}S[x(\cdot),t]\right\}Dx(\cdot)$$
$$\equiv \lim_{N\to\infty}\alpha_N\int_a^b\ldots\int_a^b\exp\left\{\frac{i}{\hbar}\mathcal{S}(x_0,\ldots,x_N,t)\right\}\times\prod_{j=1}^{N-1}dx_j. \tag{3.1}$$

where

$$\alpha_N=\left\{\frac{m}{2\pi i\hbar\Delta l}\right\}^{N/2}.$$

Next, following the method of [15], we show that $K_{a,b}(x,t)$ satisfies the Schrödinger equation and determines the boundary conditions at the end points of the interval $[a,b]$. We begin with a derivation of a recursion relation that defines $K(x,t)$. We set

$$K_N(x_N,t)\equiv\alpha_N\int_a^b\ldots\int_a^b\exp\left\{\frac{i}{\hbar}\mathcal{S}(x_0,\ldots,x_N,t)\right\}\times\prod_{j=1}^{N-1}dx_j, \tag{3.2}$$

then by the definition (3.1), $K(x,t)=\lim_{N\to\infty}K_N(x,t)$. The definition (3.2) implies the recursion relation

$$K_N(x,t)=\left\{\frac{m}{2\pi i\hbar\Delta t}\right\}^{1/2}\int_a^b\exp\left\{\frac{i}{\hbar}\left[\frac{m(x-x_{N-1})^2}{2\Delta t}-V(x)\Delta t\right]\right\}K_{N-1}(x_{N-1},t_{N-1})dx_{N-1}. \tag{3.3}$$

The following derivation is formal. A strict derivation can be constructed along the lines of [15]. We expand the function $K_{N-1}(x_{N-1},t_{N-1})$ in Eq. (3.3) in Taylor's series about x to obtain

$$K_N(x,t)=\left\{\frac{m}{2\pi i\hbar\Delta t}\right\}^{1/2}e^{-iV(x)\Delta t/\hbar}\int_a^b\exp\left\{\frac{im}{2\hbar\Delta t}(x-x_{N-1})^2\right\}\left[K_{N-1}(x,t_{N-1})-(x-x_{N-1})\times\frac{\partial K_{N-1}(x,t_{N-1})}{\partial x}+\frac{1}{2}(x-x_{N-1})^2\frac{\partial^2K_{N-1}(x,t_{N-1})}{\partial x^2}+O((x-x_{N-1})^3)\right]dx_{N-1}. \tag{3.4}$$

The integrals in Eq. (3.4) are evaluated separately for x inside the interval $[a,b]$ and on its boundaries. When x is inside the interval, the integrals become the Fresnel integrals over the entire line in the limit $\Delta t\to 0$. This recovers the Schrödinger equation inside the interval. When $x=a,b$, the first integral in Eq. (3.4) becomes in the limit $\Delta t\to 0$ the Fresnel integral over half the real line while the other integrals vanish. We obtain

$$K(a,t)=\tfrac{1}{2}K(a,t), \tag{3.5}$$

hence $K(a,t)=0$, and similarly $K(b,t)=0$. More specifically, consider the normalized nth moment of the Gaussian integral $(n=0,1,2)$

$$\alpha^n m_n(\alpha,a,b,y)=\left\{\frac{\alpha}{i\pi}\right\}^{1/2}\int_a^b(x-y)^n\exp\{-i\alpha(x-y)^2\}dx,$$

where

$$\frac{m}{2\hbar\Delta t}=\alpha.$$

We change the variable to

$$\sqrt{\alpha}(x-y)=u \tag{3.6}$$

and get

$$m_n(\alpha,a,b,y)=\left\{\frac{1}{i\pi}\right\}^{1/2}\int_{\sqrt{\alpha}(a-y)}^{\sqrt{\alpha}(b-y)}u^n\exp\{-iu^2\}du.$$

Note that the limits of integration become

$$\sqrt{\alpha}(a-y)\to-\infty, \quad \sqrt{\alpha}(b-y)\to\infty \quad \text{as} \quad \alpha\to\infty$$

so that in the limit $\Delta t\to 0$, that is, as $\alpha\to\infty$ and for $a<y<b$, we obtain

$$m_n(a,b,y)=\lim_{\alpha\to\infty} m_n(\alpha,a,b,y)$$
$$=\int_{\sqrt{\alpha}(a-y)}^{\sqrt{\alpha}(b-y)} u^n \exp\{-iu^2\}du$$
$$=\int_{-\infty}^{\infty} u^n \exp\{-iu^2\}du. \tag{3.7}$$

Note that $m_1=0$ while $m_0=m_2=1$. Now, transferring K_{n-1} to the left-hand side of Eq. (3.4), dividing by Δt, taking the limit, and applying Eq. (3.7), we recover the Schrödinger equation.

At the boundary point $y=b$, the substitution (3.6) transforms the upper limit of integration to 0. In the limit $\Delta t\to 0$, we obtain

$$m_n(a,b,b)=\lim_{\alpha\to\infty} m_n(\alpha,a,b,b)$$
$$=\lim_{\alpha\to\infty}\int_{\sqrt{\alpha}(a-b)}^{0} u^n \exp\{-iu^2\}du$$
$$=\int_{-\infty}^{0} u^n \exp\{-iu^2\}du. \tag{3.8}$$

That is, the Fresnel integrals are extended only over half the line. Thus, we obtain that the coefficient of K_{N-1} in Eq. (3.4) is

$$m_0(a,b,b)=\tfrac{1}{2},$$

while that of the first derivative of K_{N-1} is

$$\alpha^{-1}m_1(\alpha,a,b,b)\to 0$$

and that of the second derivative of K_{N-1} is

$$\alpha^{-2}m_2(\alpha,a,b,b)\to 0.$$

Thus, setting $x=b$ in Eq. (3.4) and taking the limit $\Delta t\to 0$, we obtain Eq. (3.5), which in turn implies the boundary condition Eq. (3.10).

When $a<x<b$, the derivation given in [15] leads to the Schrödinger equation. Thus

$$i\hbar\frac{\partial K(x,t)}{\partial t}=-\frac{\hbar^2}{2m}\frac{\partial^2 K(x,t)}{\partial x^2}+V(x)K(x,t) \quad \text{for} \quad a<x<b, \tag{3.9}$$

$$K(a,t)=K(b,t)=0 \quad \text{for} \quad t>0, \tag{3.10}$$

$$K(x,0)=\delta(x-x_I) \quad \text{for} \quad a<x<b. \tag{3.11}$$

In the case $a=-\infty$, $b=\infty$ every x is an internal point so that the Schrödinger equation is satisfied for all x and thus the Feynman integral (3.1) is equivalent to the Schrödinger equation (3.9) and the initial condition (3.11) on the entire real line.

This result, which was also derived by different methods in [10] and [9], shows that bounded trajectories imply in effect an infinite potential barrier on the boundary. In contrast, the Wiener integral over bounded trajectories leads to the diffusion equation with zero boundary condition and to the decay of the probability density function in the domain. This means that the boundary is absorbing. This difference between the Wiener and the Feynman integrals over the same class of functions is illustrative of the different roles that trajectories play in quantum and classical theories.

IV. FEYNMAN INTEGRALS WITH ABSORBING BOUNDARIES

Assume now that a trajectory that reaches the boundary $x=a$ or $x=b$ for the first time is instantaneously absorbed. This means that the wave function outside the interval (a,b) vanishes identically and the population inside the interval (a,b) is reduced at a rate determined by the current at the boundary, as described below. The vanishing wave function outside the interval (a,b) expresses the assumption that once outside the interval the particle no longer participates in the quantum evolution of the particles inside the interval. This may occur, for example, in the scattering of particles on a target (e.g., a nucleus). Particles absorbed in the nucleus are discounted from the scattered population. Another example is that of a particle that enters a bath, such as a photographic plate, and leaves an irreversible trace. Consequently, its quantum interaction with the particles inside the interval becomes negligible. Also in this case the population inside the interval is discounted at the rate particles are absorbed.

The absorption process at a given time t is described as the limiting process as $\Delta t\to 0$ of the propagation of a trajectory that survived in the interval $[a,b]$ till time t to a boundary point in the time interval $[t,t+\Delta t]$. In order to incorporate this behavior into the Feynman formulation, we adopt the procedure that leads to the Feynman-Kac formula for the probability density function for a diffusion process with a killing (absorption) measure (see, e.g., [16]). We consider separately the trajectories that reach the boundary in the time interval $[0,\Delta t]$, then those that survived till Δt, but reach the boundary in the time interval $[\Delta t,2\Delta t]$, and so on. In each time step, the total population of trajectories has to be discounted by the probability of the absorbed trajectories. This leads to a modified expression for the discretized Feynman integral.

First, we calculate the discretized Feynman integral in the time interval $[0,\Delta t]$,

$$\psi_1(x,\Delta t)=\left\{\frac{m}{2\pi i\hbar\Delta t}\right\}^{1/2}\int_a^b \psi_0(x_0)\exp\left\{\frac{i}{\hbar}\mathcal{S}(x_0,x,\Delta t)\right\}dx_0.$$

Therefore, the probability density of finding a trajectory at $x=a$ in the time interval $[0,\Delta t]$ is $|\psi(a,\Delta t)|^2$, and there is an analogous expression for the probability density of finding a trajectory at $x=b$ in the time interval $[0,\Delta t]$.

For simplicity, we assume that $b=0$ and we consider the interval $[-a,0]$, where $a>0$. Next, we calculate the probability density propagated from the interval $[-a,0]$ into the absorbing boundary at $x=0$ in any time interval $[t,t+\Delta t]$. We begin with an initial wave function $\psi(x,t)$ that is a polynomial in the interval $[-a,0]$,

$$Q(x,t)=\sum_{j=1}^{N} q_j(t)x^j,$$

such that $Q(-a,t)=Q(0,t)=0$ and $\psi(x,t)=0$ otherwise. The free propagation from the interval $[-a,0]$ is given by

$$\psi(y,t+\Delta t)=\sqrt{\frac{m}{2\pi i\hbar\Delta t}}\int_{-a}^{0}Q(x,t)\exp\left\{\frac{im(x-y)^2}{2\hbar\Delta t}\right\}dx.$$

The boundary condition at the left end of the support of $\psi(x,t)$ is written explicitly as

$$\sum_{j=1}^{N} q_j(t)(-a)^j=0.$$

Setting

$$\alpha=\frac{\hbar\Delta t}{m},$$

the probability density propagated freely into the absorbing boundary point $x=0$ in time Δt is given by

$$|\psi(0,t+\Delta t)|^2=\frac{1}{2\pi\alpha}\left|\int_{-a}^{0}Q(x,t)e^{ix^2/2\alpha}dx\right|^2.$$

We change variable by setting $x=\sqrt{\alpha}\xi$ to get

$$|\psi(0,t+\Delta t)|^2=\frac{1}{2\pi}\left|\int_{-a/\sqrt{\alpha}}^{0}Q(\sqrt{\alpha}\xi)e^{i\xi^2/2}d\xi\right|^2. \quad (4.1)$$

First, we evaluate the inner integral,

$$I_N=\sum_{j=1}^{N} q_j\sqrt{\alpha^j}\int_{-a/\sqrt{\alpha}}^{0}\xi^j e^{i\xi^2/2}d\xi.$$

All limits of the type

$$\lim_{\alpha\to 0+}\alpha^{-(j+1)/2}\int_{-a\sqrt{\alpha}}^{0}x^j e^{ix^2/2\alpha}dx$$

are understood in the sense

$$\lim_{\alpha\to 0+}\alpha^{-(j+1)/2}\int_{-a/\sqrt{\alpha}}^{0}x^j e^{ix^2/2\alpha}dx$$
$$=\lim_{\epsilon\to 0+}\lim_{\alpha\to 0+}\alpha^{-(j+1)/2}\int_{-a/\sqrt{\alpha}}^{0}x^j e^{(-\epsilon+i)x^2/2\alpha}dx. \quad (4.2)$$

The first term in the sum I_N gives

$$-iq_1(t)\sqrt{\alpha}\int_{-a/\sqrt{\alpha}}^{0}de^{i\xi^2/2}=-iq_1(t)\sqrt{\alpha}(1-e^{ia^2/2\alpha}).$$

The second term gives

$$-iq_2(t)a\sqrt{\alpha}e^{a^2/2\alpha}+iq_2(t)\alpha\int_{-a/\sqrt{\alpha}}^{0}e^{i\xi^2/2}d\xi.$$

Setting

$$S_j=\alpha^{j/2}\int_{-a/\sqrt{\alpha}}^{0}\xi^j e^{i\xi^2/2}d\xi,$$

integration by parts gives the recursion relation

$$S_j=i\sqrt{\alpha}(-a)^{j-1}e^{ia^2/2\alpha}+i(j-1)\alpha S_{j-2}.$$

Proceeding by induction, we find that for $j>2$

$$S_j=O(\sqrt{\alpha}e^{ia^2/2\alpha}).$$

Now, using the definition (4.2), we find that

$$\lim_{\Delta t\to 0}\frac{1}{\alpha}|\psi(0,t+\Delta t)|^2=\frac{1}{2\pi}|q_1(t)|^2.$$

Keeping in mind that

$$q_1(t)=\frac{\partial\psi(0,t)}{\partial x},$$

we can write

$$|\psi(0,t+\Delta t)|^2=\frac{\hbar\Delta t}{2\pi m}\left|\frac{\partial\psi(0,t)}{\partial x}\right|^2+o\left(\frac{\hbar\Delta t}{2\pi m}\right)\quad\text{for}\quad \alpha\ll 1. \quad (4.3)$$

Returning to the propagation from an interval $[a,b]$ to its absorbing boundaries, the Feynman trajectories in the time interval $[0,\Delta t]$ consist of those that have not reached the absorbing boundaries and those that have. We calculate the Feynman integral separately on each one of these two classes of trajectories. The integral over the first class is the one calculated in Sec. III. The integral over the latter class is the integral calculated in the above paragraphs in this section. According to our assumptions, trajectories that propagate into the absorbing boundary never return into the interval $[a,b]$ so that the Feynman integral over these trajectories is supported outside the interval. On the other hand, the Feynman integral over the bounded trajectories in the interval is supported inside the interval. Thus the two integrals are orthogonal and give rise to no interference. The Feynman integral over the bounded trajectories represents the wave function conditioned on not exiting the interval $[a,b]$ in the time interval $[0,\Delta t]$. According to Eq. (4.3) and to our assumptions, the probability defined by the Feynman integral over the trajectories that propagated into the absorbing boundary in this time interval is given by

$$P_1(\Delta t)=\lambda(a)|\psi_1(a,\Delta t)|^2+\lambda(b)|\psi_1(b,\Delta t)|^2+o(\Delta t)$$
$$=\frac{\hbar\Delta t}{2\pi m}\left\{\lambda(a)\left|\frac{\partial\psi_1(a,0)}{\partial x}\right|^2+\lambda(b)\left|\frac{\partial\psi_1(b,0)}{\partial x}\right|^2\right\}+o(\Delta t),$$

where $\lambda(a)$ and $\lambda(b)$ are the characteristic lengths at $x=a$ and $x=b$, respectively. The survival probability in this time interval is

$$S_1(\Delta t)=1-P_1(\Delta t). \tag{4.4}$$

Next, we calculate the discretized Feynman integral in the time interval $[\Delta t,2\Delta t]$ and again break it into the same classes as above. The discretized integral over the class of bounded trajectories in the interval $[a,b]$ is

$$\psi_2(x,2\Delta t)=\left\{\frac{m}{2\pi i\hbar\Delta t}\right\}^{1/2}\times\int_a^b\psi_1(x_1,\Delta t)\exp\left\{\frac{i}{\hbar}\mathcal{S}(x_1,x,\Delta t)\right\}dx_1.$$

The probability calculated from the Feynman integral over the absorbed trajectory in the time interval $[\Delta t,2\Delta t]$ is

$$P_2(2\Delta t)=\lambda(a)|\psi_2(a,2\Delta t)|^2+\lambda(b)|\psi_2(b,2\Delta t)|^2+o(\Delta t).$$

This is the conditional probability of trajectories that propagate into the absorbing boundaries in the time interval $[\Delta t,2\Delta t]$, given that they did not reach the boundaries in the previous time interval. Thus the discretized survival probability in the time interval $[0,2\Delta t]$ is

$$S_2(2\Delta t)=[1-P_1(\Delta t)][1-P_2(2\Delta t)].$$

Proceeding this way, we find that the discretized Feynman integral over the class of bounded trajectories in the time interval $[0,N\Delta t]$ is

$$\psi_N(x,N\Delta t)=\left\{\frac{m}{2\pi i\hbar\Delta t}\right\}^{1/2}\times\int_a^b\psi_{N-1}(x_{N-1},(N-1)\Delta t)\times\exp\left\{\frac{i}{\hbar}\mathcal{S}(x_{N-1},x,\Delta t)\right\}dx_{N-1}. \tag{4.5}$$

As in Eq. (3.3), we find that $\psi_N(x,N\Delta t)\to\psi(x,t)$ as $N\to\infty$, where $\psi(x,t)$ is the solution of Schrödinger's equation in (a,b) with the boundary conditions $\psi(a,t)=\psi(b,t)=0$.

The probability that propagates into the absorbing walls in the time interval $[(j-1)\Delta t,j\Delta t]$ is given by

$$P_j(j\Delta t)=\lambda(a)|\psi_j(a,j\Delta t)|^2+\lambda(b)|\psi_j(b,j\Delta t)|^2+o(\Delta t). \tag{4.6}$$

It follows that the survival probability of trajectories inside the interval is

$$S(t)=\lim_{N\to\infty}\prod_{j=1}^{N}[1-P_j(j\Delta t)]. \tag{4.7}$$

According to Eqs. (4.3) and (4.6), $P_j(j\Delta t)$ is given by

$$P_j(j\Delta t)=\frac{\hbar\Delta t}{2\pi m}\left[\lambda(a)\left|\frac{\partial}{\partial x}\psi_{j-1}(a,(j-1)t)\right|^2+\lambda(b)\left|\frac{\partial}{\partial x}\psi_{j-1}(b,(j-1)t)\right|^2+o(1)\right],$$

so that Eq. (4.7) gives the survival probability

$$S(t)=\exp\left\{-\frac{\hbar}{\pi m}\int_0^t\left[\lambda(a)\left|\frac{\partial}{\partial x}\psi(a,t')\right|^2+\lambda(b)\left|\frac{\partial}{\partial x}\psi(b,t')\right|^2\right]dt'\right\}. \tag{4.8}$$

The wave function of the trajectories that have not been absorbed by time *t* is the wave function of a particle, conditioned on not reaching the absorbing boundary by time *t*. The conditioning renormalizes the wave function inside the domain at all times and thus it remains $\psi(x,t)$. If a particle is known not to have been absorbed by time t_1, its survival probability till time $t_2>t_1$, denoted $S(t_2,t_1)$, is given by

$$S(t_2,t_1)=\exp\left\{-\frac{\hbar}{\pi m}\int_{t_1}^{t_2}\left[\lambda(a)\left|\frac{\partial}{\partial x}\psi(a,t)\right|^2+\lambda(b)\left|\frac{\partial}{\partial x}\psi(b,t)\right|^2\right]dt\right\}. \tag{4.9}$$

The function $\psi(x,t)$, which is the solution of Schrödinger's equation with homogeneous boundary conditions on the absorbing walls has the interpretation of the conditional wave function of the Feynman trajectories that have not been absorbed by time *t*. This is the wave function of the quantum particle at time *t*, given that it has not been absorbed by time *t*.

V. THE ABSORPTION CURRENT AND THE SLIT EXPERIMENT

An absorbing boundary engenders a unidirectional probability current [1] into the boundary. The simplest definition of the unidirectional current at a single absorbing point, $x=0$, in one dimension, is [see Eq. (4.8)]

$$\mathcal{J}(0,t)=\frac{d}{dt}[1-S(t)]=\lambda\left|\frac{\partial\psi(0,t)}{\partial x}\right|^2\exp\left\{-\lambda\int_0^t\left|\frac{\partial\psi(0,t')}{\partial x}\right|^2dt'\right\}. \tag{5.1}$$

In higher dimensions, we consider a domain D bounded by an absorbing boundary Γ. We denote by $\psi(\boldsymbol{x},t)$ the solution of Schrödinger's equation in D with a zero boundary condition on Γ. The survival probability is given by

$$S(t)=\exp\left\{-\lambda\int_0^t\oint_\Gamma\left|\frac{\partial\psi(\boldsymbol{x}',t')}{\partial\boldsymbol{n}}\right|^2 dS_{\boldsymbol{x}'}dt'\right\},\qquad(5.2)$$

where $\boldsymbol{n}$ is the unit outer normal to the boundary. As in Sec. IV, the function $\psi(\boldsymbol{x},t)$ is the conditional wave function of a particle, given that it has not been absorbed by time t. Generalizing the definition (5.1) to higher dimensions, the total current at the absorbing boundary is defined as

$$\begin{aligned}\mathcal{J}_\Gamma(t)&=\frac{d}{dt}[1-S(t)]\\&=\lambda\oint_\Gamma\left|\frac{\partial\psi(\boldsymbol{x},t)}{\partial\boldsymbol{n}}\right|^2_\Gamma dS_{\boldsymbol{x}'}\\&\quad\times\exp\left\{-\lambda\int_0^t\oint_\Gamma\left|\frac{\partial\psi(\boldsymbol{x}',t')}{\partial\boldsymbol{n}}\right|^2 dS'_{\boldsymbol{x}}dt'\right\}.\end{aligned}\qquad(5.3)$$

The normal component of the multidimensional probability current density at any point $\boldsymbol{x}$ on Γ is given by

$$\begin{aligned}\mathcal{J}(\boldsymbol{x},t)\cdot\boldsymbol{n}(\boldsymbol{x})|_\Gamma&=\lambda\left|\frac{\partial\psi(\boldsymbol{x},t)}{\partial\boldsymbol{n}}\right|^2_\Gamma\\&\quad\times\exp\left\{-\lambda\int_0^t\oint_\Gamma\left|\frac{\partial\psi(\boldsymbol{x}',t')}{\partial\boldsymbol{n}}\right|^2 dS_{\boldsymbol{x}'}dt'\right\}.\end{aligned}\qquad(5.4)$$

Next, we consider the slit experiment with an absorbing screen (e.g., photographic plate or a scintillation screen). In this case, unlike the usual assumption in quantum mechanics [17], the pattern that appears on the absorbing screen cannot be the squared modulus of the wave function in the entire space (with or without a finite potential), as the above analysis implies. It cannot be the modulus of the wave function with an absorbing boundary because the wave function vanishes on an absorbing boundary. According to the absorption principles, the pattern on the screen represents the probability density that propagates into the screen. This probability density is the unidirectional absorption current on the screen. Thus, the instantaneous pattern at time t is $\mathcal{J}(\boldsymbol{x},t)\cdot\boldsymbol{n}(\boldsymbol{x})|_\Gamma$ and the cumulative pattern, after the arrival of many particles, is

$$\mathcal{J}(\boldsymbol{x})\Big|_\Gamma=\int_0^\infty\mathcal{J}(\boldsymbol{x},t)\cdot\boldsymbol{n}(\boldsymbol{x})\Big|_\Gamma dt.$$

The instantaneous pattern $\mathcal{J}(\boldsymbol{x},t)\cdot\boldsymbol{n}(\boldsymbol{x})|_\Gamma$ is obtained as the histogram of points on the screen collected at time t after releasing the particle in the slit. The cumulative current density $\mathcal{J}(\boldsymbol{x})|_\Gamma$ is the histogram of points on the screen collected at all times.

We consider the following experimental setup for the slit experiment with an absorbing screen. A planar screen is placed in the plane $x=0$ and another screen is placed in the plane $x=x_0$ and it is slit along a line parallel to the z axis. Due to the invariance of the geometry of the problem in z the mathematical description of the slit is, following [17], an initial truncated Gaussian wave packet in the (x,y) plane, concentrated around the initial point, $(x_0,0)$. To describe the interference pattern on the screen, we assume it is an absorbing line on the y axis and apply the formalism developed above. According to our formalism, the pattern on the screen at time t is given by

$$\mathcal{J}(0,y,t)=\lambda\left|\frac{\partial\psi(0,y,t)}{\partial x}\right|^2\exp\left\{-\lambda\int_0^t\left|\frac{\partial\psi(0,y,t')}{\partial x}\right|^2 dt'\right\},\qquad(5.5)$$

where $\psi(x,y,t)$ is the solution of the Schrödinger equation in the half plane $x>0$ with $\psi(0,y,t)=0$ and $\psi(x,y,0)$ is the given initial packet. $\mathcal{J}(0,y,t)$ is the probability density to observe the particle at the point y on the screen at time t. The total current,

$$\mathcal{J}(y)=\int_0^\infty\mathcal{J}(0,y,t)dt,\qquad(5.6)$$

is the probability density that the particle will be ever observed at the point y on the screen. If the initial distribution of velocities in the x direction is concentrated about v_x, the density $\mathcal{J}(y)$ is approximately the same as $\mathcal{J}(0,y,\overline{t})$, where [17]

$$\overline{t}=\frac{x_0}{v_x}.\qquad(5.7)$$

In a real experiment the measurement is neither instantaneous nor infinite in time. That is, an integral over a finite time interval is observed rather than Eqs. (5.5) or (5.6). If a packet of particles is sent out Eq. (5.5) is the probability density of Feynman trajectories that propagate instantaneously at time t into the point $(0,y)$ in the screen and is seen as the density of light intensity on the (ideal) scintillation screen at time t. The function (5.6) represents the cumulative (in time) probability current density of Feynman trajectories absorbed in the wall and is seen as the density of the trace the initial packet eventually leaves on the screen (e.g., on a photographic plate).

To determine the patterns (5.5) and (5.6), we have to calculate first the two-dimensional wave function with zero boundary condition on the y axis. It can be written as

$$\psi(x,y,t)=\psi^1(x,t)\psi^2(y,t),$$

where $\psi^1(x,t)$ is the function $K(x,t)$ in Eq. (6.1) below. Note that according to our theory $\psi^1(0,\,t)=0$ because the absorbing screen is placed at $x=0$. The component $\psi^2(y,t)$ of the wave function is given by the freely propagating Gaussian slit [17]

$$\psi^2(y,t)=\int_{-\infty}^{\infty}\frac{e^{-z^2/2\sigma_y^2}}{\sqrt{2\pi i}\sigma_y}\frac{e^{-im(y-z)^2/2\hbar t}}{\sqrt{2\pi i\hbar t/m}}dz.$$

Evaluation of the integral gives

$$|\psi^2(y,t)|^2=\frac{1}{2\pi\sigma_y}\left(\frac{\hbar^2t^2}{\sigma_y^2m^2}+\sigma_y^2\right)^{-1/2}\exp\left\{-\frac{y^2}{\frac{\hbar^2t^2}{\sigma_y^2m^2}+\sigma_y^2}\right\}.$$

If $\sigma_x\ll|x_0|$, the upper limit of integration in Eq. (6.1) can be replaced by ∞ with a transcendentally small error.

According to Eq. (5.5), the instantaneous absorption rate at time t at a point $(0,y)$ on the screen is given by

$$\mathcal{J}(0,y,t)=\left|\frac{\partial K(0,t)}{\partial x}\right|^2|\psi^2(y,t)|^2, \tag{5.8}$$

where $|\partial K(0,t)/\partial x|^2$ is given in Eq. (6.2) below. Thus the pattern on the screen at time t is given by $\mathcal{J}(0,y,t)$ in Eq. (5.8).

To compare Eq. (5.8) with that given in [17], we reproduce the derivation of [17] with an initial two-dimensional Gaussian wave packet. The result gives the wave function as

$$\psi_F(x,y,t)=\psi_F^1(x,t)\psi^2(y,t)$$

and probability density at the screen at time t as

$$|\psi_F(0,y,t)|^2=\frac{1}{2\pi\sigma_x}\left(\frac{\hbar^2t^2}{\sigma_x^2m^2}+\sigma_x^2\right)^{-1/2}\times\exp\left\{-\frac{x_0^2}{\frac{\hbar^2t^2}{\sigma_x^2m^2}+\sigma_x^2}\right\}|\psi^2(y,t)|^2. \tag{5.9}$$

Comparing Eq. (5.9) with Eq. (5.8), we see that the pattern predicted by Feynman's theory differs from that in the present theory by a time-dependent factor only. The instantaneous intensity of the diffraction pattern in the absence of an absorbing screen, given in [17], is defined as $|\psi_F(0,y,t)|^2$. Thus, the introduction of an absorbing screen, according to these interpretations, gives the relative brightness as

$$\frac{\lambda\left|\frac{\partial\psi(0,y,t)}{\partial x}\right|^2}{|\psi_F(0,y,t)|^2},$$

which is a function of time only. The decay in time of the quotient reflects the fact that the absorbing screen depresses the entire wave function in time. Thus, the part of the packet that arrives later is already attenuated by the preceding absorption, relative to the unattenuated wave function in the absence of absorption.

VI. EXAMPLES

The examples include a particle between absorbing walls, and a Gaussian wave packet, representing a free particle, incident on an absorbing wall.

A. A particle between two absorbing walls

First, we consider a particle with symmetric absorbing walls at $x=0$, a and zero potential. We assume that $\lambda_{-a}=\lambda_a$. The wave function is given by

$$\psi(x,t)=\sum_{n=1}^{\infty}A_n\exp\left\{-\frac{i\hbar n^2\pi^2}{2ma^2}t\right\}\sin\frac{n\pi}{a}x.$$

It was shown in [7] that for a particle with a single energy level the wave function decays at an exponential rate proportional to the energy. However, if there are more than just one level, the exponent contains beats.

For example, for a two-level system with real coefficients, we obtain the survival probability

$$S(t)=\exp\left\{-\frac{\lambda_a\hbar}{m\pi}\left[\frac{\pi^2}{a^2}(A_k^2k^2+A_n^2n^2)t-\frac{4m(-1)^{k+n}knA_kA_n}{\hbar(n^2-k^2)}\sin\frac{\hbar(n^2-k^2)\pi^2}{2ma^2}t\right]\right\}.$$

The strongest beats occur for $k=2$, $n=1$ with frequency $\omega_{1,2}=3\hbar\pi^2/2ma^2$. Setting $A_1=A_2=\sqrt{1/2a}$ and introducing the dimensionless time $\tau=\omega_{1,2}t$, we find that the survival probability is

$$S(t)=\exp\left\{-\frac{\lambda_a}{3\pi}(5\tau-2\sin\tau)\right\}.$$

The function

$$\ln S(t)=-\frac{\lambda_a}{3\pi}(5\tau-2\sin\tau)$$

is qualitatively similar to that given in [18].

B. A wave-packet incident on an absorbing wall

Next, we consider a Gaussian-like wave packet of free particles traveling toward an absorbing wall at $x=0$ with positive mean velocity k_0. That is, the initial wave function is given by

$$\psi(x,0)=\frac{1}{a\sqrt{\pi}(1+2\exp\{-x_0^2/a^2\})}\times\left[\exp\left\{-\frac{(x-x_0)^2}{2a^2}-ik_0x\right\}-\exp\left\{-\frac{(x+x_0)^2}{2a^2}+ik_0x\right\}\right]$$

for $x \leqslant 0$. The evolution of $\psi(x,t)$ on the negative axis is given by

$$\begin{aligned}\psi(x,t)=&A(t)\int_{-\infty}^{\infty}\exp\left\{-\frac{a^2k^2}{2}+ikx-\frac{i(k^2+k_0^2)t}{2m}\right\}\\&\times\sin\left(kx_0+k_0x+\frac{kk_0}{m}t\right)dk\\=&A(t)\exp\left\{-\frac{ik_0^2t}{2m}\right\}\\&\times\left[\exp\left\{-\frac{\left(x-x_0+\frac{k_0}{m}t\right)^2}{2(a^2+it/m)}-ik_0x\right\}\right.\\&\left.-\exp\left\{-\frac{\left(x+x_0-\frac{k_0}{m}t\right)^2}{2(a^2+it/m)}+ik_0x\right\}\right], \qquad (6.1)\end{aligned}$$

where the normalization factor is given by

$$\begin{aligned}\frac{1}{A(t)}=&\sqrt{\pi\left(a^2+\frac{t^2}{a^2m^2}\right)}\\&\times\left[1+2\exp\left\{-\frac{a^2k_0^2t^2}{2(a^4m^2+t^2)}\right.\right.\\&\left.\left.-\left(a^2+\frac{t^2}{a^2m^2}\right)\left(\frac{x_0t}{m}+\frac{k_0t^2}{m^2}+x_0\right)^2\right\}\right].\end{aligned}$$

It follows that

$$\begin{aligned}\left|\frac{\partial}{\partial x}\psi(0,t)\right|^2=&A^2(t)\left[\frac{\left(x_0-\frac{k_0t}{m}\right)^2a^4m^4}{(a^4m^2+t^2)^2}\right.\\&\left.+\left(\frac{a^2m^2}{a^4m^2+t^2}+k_0\right)^2\right]\\&\times\exp\left\{-\frac{\left(x_0-\frac{k_0t}{m}\right)^2a^4m^4}{(a^4m^2+t^2)^2}\right\}, \qquad (6.2)\end{aligned}$$

hence

$$\int_0^{\infty}\left|\frac{\partial}{\partial x}\psi(0,t)\right|^2dt<\infty. \qquad (6.3)$$

Thus

$$R=S(\infty)>0,$$

that is, the wave packet is only partially absorbed. This means that the ''reflected'' wave consists of trajectories that turned around before propagating past the absorbing wall. The absorption occurs when the trajectory propagates into the medium inside the wall. The discount of the wave function occurs when the packet is at the wall, as can be seen from Eqs. (6.2) and (6.3). Thus R plays the role of a *reflection coefficient*. This is neither the usual reflection coefficient for a finite potential barrier nor that for an infinite barrier. The reflection coefficient is a function of the packet group velocity k_0, the width of the packet a, its initial distance from the absorbing screen x_0, the parameter λ, and its mass m. This dependence is experimentally measurable.

VII. DISCUSSION AND SUMMARY

In this paper a theory of absorption of quantum particles in a surface is proposed. The theory is based on an analog of absorption in diffusion theory as expressed in the Wiener integral. The path-integral approach to absorption of a quantum particle differs from absorption in diffusion theory in that the probability propagated into the absorbing surface per unit time has to be discounted from the overall surviving population at each time step. This is due to the fact, that unlike in diffusion theory, where an infinite killing rate in a domain leads to absorption on the boundary of the domain, in quantum theory an infinite real or complex potential leads to total reflection in the boundary. There is no analog in the Schrödinger equation to the absorbing boundary condition in the Fokker-Planck equation.

While a homogeneous boundary condition for the Fokker-Planck equation gives rise to absorption, the same condition for the Schrödinger equation leads to total reflection. There is neither a boundary condition nor a potential for the Schrödinger equation that leads to absorption in a boundary of a domain. The discounting procedure is analogous to that used in the derivation of the Feynman-Kac formula for diffusion with a killing measure.

In this derivation the Wiener integral is discounted by the probability of being killed at every time step. We observe that according to Eq. (4.4) there is conservation of probability: the probability of the absorbed Feynman trajectories and that of the surviving trajectories sum to 1. This is the result of our postulate that the Feynman integrals over the two classes of trajectories have disjoint supports, that is, the absorbed trajectories never return to the interval $[a,b]$. This conservation of probability persists for all times. This result is different from that obtained in decoherent state theory [19]. The main result of this paper is an expression for the survival probability of a quantum particle in the presence of an ideal absorbing wall. The survival probability $S(t)$ is the probability obtained by repeating the experiment of observing the particle between the absorbing boundaries at time t and constructing a histogram of the number of times the particle is observed. This probability is not a quantum-mechanical quantity in the sense that it is not the integral of the squared modulus of a probability amplitude defined by Schrödinger's equation. The wave function of the particle at time t, given that it has not been absorbed by that time, is the wave function $\psi(x,t)$ defined by Schrödinger's equation inside the given domain with reflecting boundary conditions.

That is, if the absorbing boundary represents a detector, the wave function of the particle is $\psi(x,t)$ as long as the particle has not been detected. Thus $\psi(x,t)$ is the conditional wave function of unabsorbed particles and is normalized to 1. The unconditional wave function in the domain, denoted $\Psi(x,t)$, is normalized to the survival probability $S(t)$. To understand the difference between the conditional and the unconditional wave function consider the following experiment. N particles are released at a point in a domain D whose boundary is absorbing. A subdomain $D' \subset D$ is illuminated at time t after the particles are released and the number of particles observed in D', denoted $N(t)$, is recorded. The number of particles absorbed in the wall by time t, denoted $\tilde{N}(t)$, is also recorded. Then

$$\lim_{N\to\infty} \frac{N(t)}{N} = \int_{D'} |\Psi(x,t)|^2 dx,$$

$$\lim_{N\to\infty} \frac{\tilde{N}(t)}{N} = 1 - S(t),$$

$$\lim_{N\to\infty} \frac{N(t)}{N-\tilde{N}(t)} = \int_{D} |\psi(x,t)|^2 dx.$$

Thus, we can write

$$|\Psi(x,t)|^2 = S(t)|\psi(x,t)|^2.$$

The process of absorption of a quantum particle can be illustrated by a packet that hits, for example, a scintillation screen. At the moment a particle hits the screen it is absorbed in the sense that it is no longer a quantum particle. Its trajectory is discounted from the surviving trajectories of the packet. This is also the case for any other detector that absorbs particles. The surviving trajectories, those that have not reached the absorbing boundary so far, give rise to a reflected wave, as if the absorbing boundary were an infinite potential wall. This fact becomes apparent not from a solution of a wave equation, but rather from the calculation of the Feynman integral over a class of bounded trajectories. The example of a particle incident on an absorbing wall demonstrates the expected phenomenon of backflow at a detector.

Our derivation does not start with a Hamiltonian, but rather with an action of trajectories in a restricted class. Quantum mechanics without absorption is recovered from our formalism when the absorbing boundaries are moved to infinity or when the absorption constant λ vanishes. A detailed theory of λ can be expected to involve the atomic detail of the absorber. In contrast, our theory involves the trajectories of the particle before they hit the absorbing wall so that λ is an external input into our theory.

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