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Conditional time delay in scattering theory

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Abstract. We give a general and mathematically precise definition of the notion of conditional time delay in scattering theory i.e., a notion of time delay for a given condition of observation of the scattered particle. A formula, generalising the Eisenbud-Wigner time delay formula, is derived. The basic concept entering in the definition of the conditional time delay is that of conditional sojourn time. Although conditional sojourn times cannot be uniquely defined in quantum mechanics because of the uncertainty principle, we show that conditional time delays admit a well defined probabilistic interpretation in the limit of infinitly extended spatial regions. Some comments are presented in relation with the tunneling time problem.

1. Introduction

The concept of sojourn time has been successfully applied in non relativistic quantum scattering theory to give a general, physically transparent and mathematically precise definition of the global time delay and to study its relation to the energy derivative of phase shifts. More precisely, if ψ_t denotes the (normalized and square integrable) wave function at time t of a scattering state which is asymptotic to a free evolving state φ_t in the remote past ($\lim \| \psi_t - \varphi_t \| = 0$ in the Hilbert space norm as $t \to -\infty$), then the real number ($\varphi \equiv \varphi_{t=0}$)

$$T(B_r, \varphi) \equiv \int_{-\infty}^{\infty} dt \, \| F_{B_r} \psi_t \|^2 \tag{1.1}$$

where F_{B_r} denotes the projection operator onto the set of states localized in the ball B_r of radius r, centered at the origin in configuration space, may be interpreted as the average total time spent by this state, during its complete evolution, inside the ball B_r and is

usually called the sojourn time (or transit, or residence, or dwell time) of ψ_t in B_r (see the review paper [1]). In a similar way, one introduces for comparison the free sojourn time

$$T^0_{\text{in}}(B_r,\varphi) \equiv \int_{-\infty}^{\infty} dt \,\| F_{B_r}\varphi_t \|^2 \tag{1.2}$$

associated to the (free evolving) incoming asymptotic state φ_t. The difference between these two quantities represents then the time delay

$$\tau(B_r,\varphi) \equiv T(B_r,\varphi) - T^0_{\text{in}}(B_r,\varphi) \tag{1.3}$$

for the ball B_r and for a scattering initiated in the state φ. The time delay for the initial state φ is defined as the limit of $\tau(B_r,\varphi)$ as $r \to \infty$ [1]. We write for it

$$\tau(\varphi) \equiv \lim_{r\to\infty} \tau(B_r,\varphi). \tag{1.4}$$

A large litterature is devoted to the proof of the existence of the limit (1.4) and its identity to the Eisenbud-Wigner time delay formula ([1],[3]-[11])

$$\tau_{\text{E-W}}(\varphi) \equiv (\varphi, \tau_{\text{E-W}}\varphi) \tag{1.5}$$

where $\tau_{\text{E-W}}$ is the Eisenbud-Wigner time delay operator with energy shell components

$$\tau_{\text{E-W}}(E) \equiv -iS^\dagger(E)\frac{\partial S(E)}{\partial E} \tag{1.6}$$

and $S(E)$ is the scattering operator at energy E, acting on square integrable wave functions of the angular variables in momentum space. Formula (1.5),(1.6) generalize the classical formula of Eisenbud and Wigner asserting that, for scattering by a spherically symmetric potential in a given partial wave subspace, the time delay is expressed by the derivative of the phase shift with respect to energy (see [12],[13] but also [1]).

However, the time delay (1.3),(1.4) is a global quantity. Indeed, its calculation involves the scattered wave in all directions i.e., with no specification of the conditions of observation of the scattered particle. Another possibility is to introduce a notion of time delay more appropriate for scattering observed by counters in a differential cross-section measurement i.e., a notion of time delay from a given direction into a given direction of observation of the scattered particle, namely an angular time delay. The idea for this type of time delay apparently was present in the original work of Eisenbud and Wigner [12],[13] and has since been studied by number of authors (see [14] and references therein). Under

[1] The limit (1.4) for the time delay can exist, in general, only for sequences of dilated balls. If the limit exists, it also depends on the arbitrary choice of the dilation center of the balls [2]. Throughout all this paper we shall only consider, for simplicity, balls centered at the origin.

certain circumstances it has been found that the angular time delay $\tau_E(\hat{k}_1, \hat{k}_2)$ for an initial direction $\hat{k}_1$ and a final direction $\hat{k}_2$ (at fixed energy E) is given by the derivative of the argument of the corresponding S-matrix element

$$\tau_E(\hat{k}_1, \hat{k}_2) = \frac{d}{dE} \arg(\hat{k}_2|S(E)|\hat{k}_1). \tag{1.7}$$

However, unlike the global time delay, the angular time delay has not received until now a general and mathematically precise definition.

The main purpouse of the present paper is to provide a general, mathematically precise and physically transparent definition of the concept of conditional time delay $\tau^F(\varphi)$ i.e., the time delay corresponding to an initial state φ and for a scattered state which is ultimately observed in some arbitrary subspace of the space of scattering states, specified by the range of a given projection operator F. For instance, if F is the projection operator onto the subspace of states with momentum lying in the cone $C(\hat{k}_2, \alpha) \equiv \{\vec{k} \in \mathbb{R}^3 | \vec{k} \cdot \hat{k}_2 \geq \alpha |\vec{k}|\}$, where $|\hat{k}_2| = 1$ and $0 < \alpha \leq 1$, then (according to Dollard's scattering into cones [15]) $\tau^F(\varphi)$ will be the time delay for an initial state φ and for a scattering state found in the cone $C(\hat{k}_2, \alpha)$ in configuration space as $t \to \infty$. Passing then to the limit of an incoming plane wave with direction $\hat{k}_1$ and of a cone of vanishing apex-angle (i.e., $\alpha \to 1$), we recover in section 4 the angular time delay (1.7).

The basic concept entering in the definition of the global time delay is that of sojourn time. In the same way, we shall see that the basic concept entering in the definition of the conditional time delay is that of conditional sojourn time i.e., a concept of sojourn time condititonal to a given observation of the scattered particle. To do this we shall proceed as follows. In section 2 we consider the one-dimensional motion of a classical scattering particle with initial conditions distributed by some probability law in phase space. In this particular context, we shall define the average sojourn times for transmitted and reflected trajectories separately. Transmission and reflection time delays will then be defined with respect to suitable choices of the free reference times. This section should be considered as a preparative for section 3 where we construct the quantum transmission and reflection sojourn times as the natural quantum analogues of the corresponding classical quantities. The main conceptual difficulty that we shall encounter in this generalization is related to the non-existence, in quantum mechanics, of analogues of classical objects such as joint probability distributions (and thus conditional probabilities) for non commuting observables. As a consequence, due to Heisenberg's uncertainty principle, conditional sojourn times with a proper probabilistic interpretation cannot be defined, in general, in quantum mechanics. However, this difficulty will not play a crucial role as long as one is interested in the time delay limit. Some comments will be presented in relation with the tunneling time controversy. Section 4 is devoted to the natural generalization of the results of section 3 to the case of a three-dimensional scattering and for more general conditions of observation of the scattering particle. A formula, generalizing the Eisenbud-Wigner time delay formula (1.5),(1.6), will be derived. Under suitable assumptions it will be shown that this formula specializes to the angular time delay formula (1.7).

2. One-dimensional classical scattering

We consider in this section the simple system constituted by a one-dimensional classical particle of mass m moving in an external conservative force field $F(x) = -dV(x)/dx$. We shall assume for simplicity that the force has a finite range (x_1, x_2) (i.e., $V(x) = 0$ for $x \leq x_1$ and $x \geq x_2$). The states of such a single particle system are points $(x,p) \in \mathbb{R}^2$ representing the position and the momentum of the particle. The free and interacting dynamical transformations are given by

$$\begin{aligned} \Phi_t^0 &: (x,p) \longmapsto (x+pt, p) \\ \Phi_t &: (x,p) \longmapsto (x(t), p(t)) \end{aligned} \tag{2.1}$$

where $p(t) = m dx(t)/dt$ and $x(t)$ is the unique solution of the equation $m d^2x(t)/dt^2 = F(x(t))$ with initial conditions $x(0) = x$ and $dx/dt(0) = p/m$ [16]. In the usual way, we define the "Möller transformations"

$$\Omega_\pm \equiv \lim_{t \to \pm\infty} \Phi_{-t} \circ \Phi_t^0 \tag{2.2}$$

and the scattering transformation

$$S \equiv \Omega_+^{-1} \circ \Omega_- \tag{2.3}$$

where $\circ$ denotes compositions of maps and we assume asymptotic completeness [16]. An important property of the scattering transformation (2.3) is that it commutes with the free evolution i.e.,

$$S \circ \Phi_t^0 = \Phi_t^0 \circ S. \tag{2.4}$$

Let us now suppose that we have an ensemble of initial conditions $(x_0, p_0) \in \mathbb{R}^2$, at time $t = 0$, described by a probability distribution f such that $\int_{-\infty}^{\infty} dx_0 \int_{-\infty}^{\infty} dp_0 f(x_0, p_0) = 1$. We also assume that the particles come from the left i.e., $f(x_0, p_0) = 0$ for all $x_0 \in \mathbb{R}$ if $p_0 \leq 0$. The scattering state at time t, associated with the initial condition (x_0, p_0), is $\Phi_t \circ \Omega_-(x_0, p_0)$. Thus, the probability $P_t(\Sigma, f)$ of finding, at time t, a particle in a volume $\Sigma \subset \mathbb{R}^2$ in phase space is given by

$$P_t(\Sigma, f) = \int_{-\infty}^{\infty} dx_0 \int_{-\infty}^{\infty} dp_0 \, X_\Sigma \circ \Phi_t \circ \Omega_-(x_0, p_0) f(x_0, p_0) \tag{2.5}$$

where X_Σ is the characteristic function of the volume Σ ($X_\Sigma(x,p) = 1$ if $(x,p) \in \Sigma$ and $X_\Sigma(x,p) = 0$ otherwise). Making the change of variables $(x,p) = \Phi_t \circ \Omega_-(x_0, p_0)$ and using the well known fact that the transformations (2.1)-(2.3) are measure preserving [16], the probability (2.5) may be rewritten into the form

$$P_t(\Sigma, f) = \int_{-\infty}^{\infty} dx \int_{-\infty}^{\infty} dp \, X_\Sigma(x,p) f_t(x,p) \equiv \langle X_\Sigma \rangle_{f_t} \tag{2.6}$$

where $f_t(x,p) \equiv f \circ \Omega_-^{-1} \circ \Phi_{-t}(x,p)$ is the probability (distribution) of finding a particle, at time t, with position x and momentum p. Let now X_{B_r} be the characteristic function of $\{x | x \in (-r,r)\} \times \mathbf{R}$ where $(-r,r)$ is a finite interval containing the support of the potential. Then, $P_t(B_r,f) = \langle X_{B_r} \rangle_{f_t}$ is the probability of finding, at time t, a particle in the interval $(-r,r)$. The average time spent in $(-r,r)$ during a complete evolution, for the initial distribution f, may then be defined as the integral

$$T(B_r,f) \equiv \int_{-\infty}^{\infty} dt\, P_t(B_r,f). \tag{2.7}$$

In the same way, we define the free reference average time $T^0_{\text{in}}(B_r,f)$ associated with the (free evolving) incoming asymptotic states $\Phi^0_t(x_0,p_0)$ by

$$T^0_{\text{in}}(B_r,f) \equiv \int_{-\infty}^{\infty} dt\, P^0_{\text{in},t}(B_r,f) \tag{2.8}$$

where $P^0_{\text{in},t}(B_r,f) = \langle X_{B_r} \rangle_{f^0_t}$ and $f^0_t \equiv f \circ \Phi^0_{-t}$. The average global time delay, for the initial distribution f, may then be defined as the limit

$$\tau(f) \equiv \lim_{r\to\infty} \left(T(B_r,f) - T^0_{\text{in}}(B_r,f) \right). \tag{2.9}$$

However, since the scattering states $\Phi_t \circ \Omega_-(x_0,p_0)$ are as closely associated with the outgoing asymptotic states $\Phi^0_t \circ S(x_0,p_0)$ as they are with the incoming ones, an equally reasonable definition for the time delay is

$$\tau(f) \equiv \lim_{r\to\infty} \left(T(B_r,f) - T^0_{\text{out}}(B_r,f) \right) \tag{2.10}$$

where $T^0_{\text{out}}(B_r,f)$ is the free reference average time associated with the outgoing asymptotic states $\Phi^0_t \circ S(x_0,p_0)$ i.e.,

$$T^0_{\text{out}}(B_r,f) \equiv \int_{-\infty}^{\infty} dt\, P^0_{\text{out},t}(B_r,f) \tag{2.11}$$

with

$$\begin{aligned} P^0_{\text{out},t}(B_r,f) &= \int_{-\infty}^{\infty} dx_0 \int_{-\infty}^{\infty} dp_0\, X_{B_r} \circ \Phi^0_t \circ S(x_0,p_0) f(x_0,p_0) \\ &= \int_{-\infty}^{\infty} dx \int_{-\infty}^{\infty} dp\, X_{B_r}(x,p) f^0_t \circ S^{-1}(x,p) = \langle X_{B_r} \rangle_{f^0_t \circ S^{-1}} \end{aligned} \tag{2.12}$$

where for the second equality in (2.12) we have made the change of variables $(x,p) = \Phi^0_t \circ S(x_0,p_0)$. However, since the scattering transformation is energy conserving, we have[2]

$$T^0_{\text{in}}(B_r,f) = T^0_{\text{out}}(B_r,f). \tag{2.13}$$

[2] In more than one dimension the equality (2.13) still holds for spherically symmetric potentials and in general it is to be replaced by $T^0_{\text{in}}(B_r,f) = T^0_{\text{out}}(B_r,f) + O(r^{-1})$; see for instance [10].

In other terms, the free reference average time is independent of the choice of incoming or outgoing asymptotic states and the definitions (2.9) and (2.10) are in fact equivalents.

A scattering particle coming from the left is transmitted (alternatively, reflected) if its outgoing momentum is positive (alternatively, negative). Thus, the transmission (+) and reflection (−) probabilities $P^{\pm}(f)$, for the initial distribution f, are given by

$$P^{\pm}(f) = \int_{-\infty}^{\infty} dx_0 \int_{-\infty}^{\infty} dp_0 \, X^{\pm} \circ S(x_0,p_0) f(x_0,p_0) \equiv \int_{-\infty}^{\infty} dx_0 \int_{-\infty}^{\infty} dp_0 \, f^{\pm}(x_0,p_0) \qquad (2.14)$$

where $X^{\pm}(x,p) \equiv \Theta(\pm p)$ and Θ is the usual Heaviside step function. In view of defining the average time spent in $(-r,r)$, conditional to the fact that the particles are ultimately transmitted (alternatively, reflected), we consider the time-dependent characteristic functions

$$X_t^{\pm} \equiv X^{\pm} \circ S \circ \Omega_-^{-1} \circ \Phi_{-t} \qquad (2.15)$$

and we observe that

$$\langle X_t^{\pm} \rangle_{f_t} = P^{\pm}(f). \qquad (2.16)$$

The conditional probabilities $P_t(B_r|\pm,f)$ of finding a particle in $(-r,r)$ at time t, knowing that the particles will be ultimately transmitted (alternatively, reflected) are then given by

$$P_t(B_r|\pm,f) = \frac{\langle X_t^{\pm} X_r \rangle_{f_t}}{P^{\pm}(f)} \qquad (2.17)$$

and the average sojourn times $T^{\pm}(B_r,f)$ in $(-r,r)$, associated to the initial distribution f, for transmitted (alternatively, reflected) particles may be defined as the integral

$$T^{\pm}(B_r,f) = \int_{-\infty}^{\infty} dt \, P_t(B_r|\pm,f). \qquad (2.18)$$

Clearly, for the conditional sojourn times (2.18) we have the conditional average

$$T(B_r,f) = P^{+}(f)T^{+}(B_r,f) + P^{-}(f)T^{-}(B_r,f). \qquad (2.19)$$

since $X^{+} + X^{-} = I$. The next step is to define, for comparison, free sojourn times associated with the outgoing asymptotic states, for transmitted and reflected particles separately[3]. For this, we notice that for a free evolution $X_t^{\pm}$ is simply to be replaced

[3] It is worth noting that, countrary to the case of the global time delay (2.9),(2.10), the choice of outgoing asymptotic states (instead of incoming ones) in the definition of free reference times for transmitted and reflected particles separately is necessary in order to correctly substract the linear divergence in (2.18), as $r \to \infty$ (see the explicit calculation in appendix A).

by $X^{\pm}$ and we have $\langle X^{\pm}\rangle_{f_t^0\circ S^{-1}} = P^{\pm}(f)$. The average free reference sojourn times for transmitted (alternatively, reflected) particles are then given by

$$T_{\text{out}}^{0,\pm}(B_r, f) = \int_{-\infty}^{\infty} dt\, P_{\text{out},t}^{0}(B_r|\pm, f) \tag{2.20}$$

where $P_{\text{out},t}^{0}(B_r|\pm, f) = \langle X^{\pm} X_{B_r}\rangle_{f_t^0\circ S^{-1}}/P^{\pm}(f)$. The time delays $\tau^{\pm}(f)$, for the initial distribution f, conditional to the fact that the particles are transmitted (alternatively, reflected), may then be defined as the limit

$$\tau^{\pm}(f) \equiv \lim_{r\to\infty} \left(T^{\pm}(B_r, f) - T_{\text{out}}^{0,\pm}(B_r, f)\right) \tag{2.21}$$

and the global (unconditional) time delay (2.9),(2.10) is given by

$$\tau(f) = P^{+}(f)\tau^{+}(f) + P^{-}(f)\tau^{-}(f). \tag{2.22}$$

An explicit calculation yields (see appendix A)

$$\tau^{\pm}(f) = P^{\pm}(f)^{-1} \int_0^{\infty} dE\, f^{\pm}(E) \frac{d\alpha_{\text{cl}}^{\pm}(E)}{dE}. \tag{2.23}$$

where $E = p_0^2/2m$, $f^{\pm}(E) \equiv \sqrt{\frac{m}{2E}} \int_{-\infty}^{\infty} dx_0 f^{\pm}(x_0, \sqrt{2mE})$ and $\alpha_{\text{cl}}^{\pm}(E)$ are the generators of the scattering transformation (2.3), corresponding to the so-called quasiclassical approximations for the quantum-mechanical phase shifts (see [17] and references therein).

3. One-dimensional quantum scattering

We consider in this section the quantum-mechanical generalisation of the classical description presented in section 2. Let $U_t^0 = \exp(-iH_0 t)$ and $U_t = \exp(-iHt)$ be the free and total evolution on the Hilbert space $\mathcal{H} \equiv L^2(\mathbb{R})$ of quantum states, with self-adjoint generators $H_0 = -(1/2m)d^2/dx^2$ and $H = -(1/2m)d^2/dx^2 + V(x)$ being respectively the free and total hamiltonian (m is the mass of the particle and we have set $\hbar = 1$). The potential V is such that the wave operators $\Omega_{\pm} \equiv s-\lim_{t\to\infty} U_{\pm t}^{\dagger} U_{\pm t}^{0}$ exist and are complete and the scattering operator $S \equiv \Omega_{+}^{\dagger}\Omega_{-}$ is unitary [16]. For sake of simplicity we shall assume, as in section 2, that the potential has finite range (x_1, x_2).

According to the statistical interpretation of quantum theory, the random variables of probability theory correspond to the observables of quantum theory and the probability measures to the states. The correspondance between the classical objects defined in section 2 and their quantum mechanical analogues is then given by the following dictionary

$$\begin{aligned}
\langle(\ \cdot\ )\rangle_{f_t} &\longleftrightarrow (\psi_t, (\ \cdot\ )\psi_t)\\
\langle(\ \cdot\ )\rangle_{f_t^0} &\longleftrightarrow (\varphi_t, (\ \cdot\ )\varphi_t)\\
\langle(\ \cdot\ )\rangle_{f_t^0\circ S^{-1}} &\longleftrightarrow (S\varphi_t, (\ \cdot\ )S\varphi_t)\\
X_{B_r} &\longleftrightarrow F_{B_r}\\
X_t^{\pm} &\longleftrightarrow F_t^{\pm} \equiv U_t\Omega_{-}S^{\dagger}F^{\pm}S\Omega_{-}^{\dagger}U_t^{\dagger}
\end{aligned} \tag{3.1}$$

where $\psi_t \equiv U_t\Omega_-\varphi$ is the scattering state at time t, for a scattering initiated in the state φ, $\varphi_t \equiv U_t^0\varphi$ is the (free evolving) incoming asymptotic state ($\lim \| \psi_t - \varphi_t \| = 0$ as $t \to -\infty$) and $S\varphi_t = U_t^0 S\varphi$ is the (free evolving) outgoing asymptotic state ($\lim \| \psi_t - S\varphi_t \| = 0$ as $t \to \infty$). F_{B_r} is the projection operator onto the set of states localized in the spatial interval $(-r, r)$ and we have $(\psi_t, F_{B_r}\psi_t) = \| F_{B_r}\psi_t \|^2 \equiv P_t(B_r, \varphi)$ which is the probability of finding the particle in $(-r, r)$, at time t, for the initial state φ. The quantum analogue of (2.16) is given by

$$(\psi_t, F_t^{\pm}\psi_t) = (\varphi, \Omega_-^{\dagger} U_t^{\dagger} F_t^{\pm} U_t \Omega_- \varphi) = (\varphi, S^{\dagger} F^{\pm} S\varphi) = \| F^{\pm} S\varphi \|^2 \equiv P^{\pm}(\varphi) \tag{3.2}$$

where $F^{\pm} \equiv \Theta(\pm P)$ (P is the momentum operator) are the projection operators onto the set of states of positive (alternatively, negative) momentum.

We come now to the crucial point of giving the quantum analogue of the conditional probabilities (2.17). Unfortunately, countrary to the classical random variables X_{B_r} and $X_t^{\pm}$, the projection operators F_{B_r} and $F_t^{\pm}$ do not commute i.e., they correspond to uncompatible observables. Now, it is a well known fact that no genuine joint probabilities exist in quantum mechanics for non commuting observables. Despite this fundamental difficulty let us consider the following auxiliary function

$$W_t(B_r, \pm; \varphi) \equiv \left(\psi_t, \frac{1}{2}(F_t^{\pm} F_{B_r} + F_{B_r} F_t^{\pm})\psi_t \right). \tag{3.3}$$

It is then an easy matter to check that (3.3) obeys to the relations we would expect from such a joint probability i.e.,

(i) $P_t(B_r, \varphi) = W_t(B_r, +; \varphi) + W_t(B_r, -; \varphi)$,

(ii) $P^{\pm}(\varphi) = W_t(B_r, \pm; \varphi) + W_t(\overline{B_r}, \pm; \varphi)$, $\quad \overline{B_r} \equiv \mathbb{R} \backslash B_r$.

Moreover, although (3.3) does not possess a proper probabilistic interpretation as is clear from the fact that it may take negative values, in the limit $r \to \infty$, we have $s\text{-}\lim_{r\to\infty} F_{B_r} = I$ and thus

$$\lim_{r\to\infty} W_t(B_r, \pm; \varphi) = P^{\pm}(\varphi) \geq 0. \tag{3.4}$$

In other terms, in this limit, the observables F_{B_r} and $F_t^{\pm}$ become compatibles and (3.3) becomes non negative i.e., it recover a consistent joint probability interpretation. Thus, keeping in mind that at the end we shall consider the time delay limit $r \to \infty$, we define the natural quantum analogues (in the sense of (i),(ii)) of the classical transmission and reflection sojourn times (2.18) by

$$\begin{aligned} T^{\pm}(B_r, \varphi) &\equiv P^{\pm}(\varphi)^{-1} \int_{-\infty}^{\infty} dt \left(\psi_t, \frac{1}{2}(F_t^{\pm} F_{B_r} + F_{B_r} F_t^{\pm})\psi_t \right) \\ &= P^{\pm}(\varphi)^{-1} \int_{-\infty}^{\infty} dt \, \mathrm{Re}(\psi_t, F_t^{\pm} F_{B_r} \psi_t) = \mathrm{Re}\left(\frac{(\varphi, S^{\dagger} F^{\pm} S T_{B_r} \varphi)}{\| F^{\pm} S\varphi \|^2} \right) \end{aligned} \tag{3.5}$$

where $T_{B_r} \equiv \int_{-\infty}^{\infty} dt\, \Omega_-^\dagger U_t^\dagger F_{B_r} U_t \Omega_- = \int_{-\infty}^{\infty} dt\, U_t^{0\dagger} \Omega_-^\dagger F_{B_r} \Omega_- U_t^{0\dagger}$ is the sojourn time operator. Notice that, because of (i), we immediatly obtain

$$T(B_r,\varphi) = P^+(\varphi)T^+(B_r,\varphi) + P^-(\varphi)T^-(B_r,\varphi) \tag{3.6}$$

where $T(B_r,\varphi) = (\varphi, T_{B_r}\varphi)$ is the global sojourn time (1.1). According to (2.20), transmission (alternatively, reflection) free reference sojourn times are given by

$$\begin{aligned} T_{\text{out}}^{0,\pm}(B_r,\varphi) &\equiv P^\pm(\varphi)^{-1} \int_{-\infty}^{\infty} dt \left(S\varphi_t, \frac{1}{2}(F^\pm F_{B_r} + F_{B_r} F^\pm) S\varphi_t \right) \\ &= P^\pm(\varphi)^{-1} \int_{-\infty}^{\infty} dt\, \text{Re}(S\varphi_t, F^\pm F_{B_r} S\varphi_t) = \text{Re}\left(\frac{(\varphi, S^\dagger F^\pm S(S^\dagger T_{B_r}^0 S)\varphi)}{\| F^\pm S\varphi \|^2} \right) \end{aligned} \tag{3.7}$$

where $T_{B_r}^0 \equiv \int_{-\infty}^{\infty} dt\, U_t^{0\dagger} F_{B_r} U_t^0$ is the free sojourn time operator. Then, the time delays for the initial state φ conditional to the fact that the particle is ultimately transmitted (alternatively, reflected) may be defined as the limit

$$\tau^\pm(\varphi) \equiv \lim_{r\to\infty} \left(T^\pm(B_r,\varphi) - T_{\text{out}}^{0,\pm}(B_r,\varphi) \right) \tag{3.8}$$

and we have the average

$$\tau(\varphi) = P^+(\varphi)\tau^+(\varphi) + P^-(\varphi)\tau^-(\varphi) \tag{3.9}$$

where $\tau(\varphi)$ is the global time delay (1.4)[4].

For a sufficiently well behaved incoming state φ, describing a particle approaching the potential from the left, an explicit calculation yields (see appendix B)

$$\tau^\pm(\varphi) = P^\pm(\varphi)^{-1} \int_0^{\infty} dE\, |A^\pm(E)\varphi(E)|^2 \frac{d\alpha^\pm(E)}{dE} \tag{3.10}$$

where $A^\pm(E) = |A^\pm(E)| \exp(i\alpha^\pm(E))$ are respectively the transmission and reflection coefficients at energy E.

[4] Notice that, as for the classical case, the free sojourn times $T_{\text{in}}^0(B_r,\varphi) = (\varphi, T_{B_r}^0\varphi)$ and $T_{\text{out}}^0(B_r,\varphi) = (\varphi, S^\dagger T_{B_r}^0 S\varphi)$ are the same for spherically symmetric potentials (see (4.5)) and in general as $r \to \infty$; see for instance [18].

Remarks

1) It is worth emphasizing that (3.3) is a natural choice only in view of the limit $r \to \infty$ (because of (3.4)). If r is kept finite, it may be preferable, instead of (3.3), to keep the non-negativity along with (i) and give up (ii) by considering

$$W_t(B_r, \pm; \varphi) = \| F_t^{\pm} F_{B_r} \psi_t \|^2 . \tag{3.11}$$

For this choice $T^{\pm}(B_r, \varphi)$ is still a (real) well defined quantity though it does not have a simple expression like (3.5). Another possibility is to keep the non-negativity along with (ii) and give up (i) by considering

$$W_t(B_r, \pm; \varphi) = \| F_{B_r} F_t^{\pm} \psi_t \|^2 . \tag{3.12}$$

This gives

$$T^{\pm}(B_r, \varphi) = P^{\pm}(\varphi)^{-1} T(B_r, S^{\dagger} F^{\pm} S \varphi) \equiv T(B_r, \varphi^{\pm}) \tag{3.13}$$

i.e., the global sojourn time for the normalized part $\varphi^{\pm} \equiv P^{\pm}(\varphi)^{-\frac{1}{2}} S^{\dagger} F^{\pm} S \varphi$ of the initial wave packet φ which is ultimately transmitted (alternatively reflected). This is the definition taken in [19] for transmission and reflection sojourn (dwell) times.

2) We observe that the time delay formula (3.10) is the direct quantum generalisation of the classical formula (2.23) in the sense of the correspondances

$$\begin{aligned} f^{\pm}(E) &\longleftrightarrow |A^{\pm}(E)\varphi(E)|^2 \\ \alpha_{\mathrm{cl}}^{\pm}(E) &\longleftrightarrow \alpha^{\pm}(E). \end{aligned} \tag{3.14}$$

3) In the limit of an incoming state approaching a plane wave, formula (3.10) yelds the (here one-dimensional) angular time delay formula (1.7). However, (3.10) is valid for general (sufficiently well behaved) incoming states φ and in that sense it is more general than (1.7).

4) A different definition for transmission and reflection time delays, using the concept of sojourn time, has been proposed in [20]. However, countrary to our case, their approach is drastically restricted to one-dimensional scattering and yields, for these times, divergent expressions in the limit $r \to \infty$.

5) The recent controversy on tunneling times has evolved around the question of finding a well-defined and universal quantity giving the average time spent by a transmitted (alternatively, reflected) quantum (one-dimensional) particle in a finite interval containing the range of the potential (see the review papers [21],[22]). According to the present analysis, the tunneling time question may simply be restated as follows: what is the quantum analogue of the (classical) random variable $X_t^{\pm} X_{B_r}$? The question is clearly an hill-defined one since the projection operators $F_t^{\pm}$ and F_{B_r}, which are respectively the quantum analogues of the characteristic functions $X_t^{\pm}$ and X_{B_r}, correspond to uncompatible observables

(i.e., they do not commute). This simply means that conditional sojourn times cannot be uniquely defined in quantum mechanics because of the uncertainty principle. In other terms, the tunneling time question is a classical question which does not admit a general answer in the realm of quantum mechanics. However, as far as one is concerned with the notion of time delay, the situation is different. Indeed, in the limit $r \to \infty$, the observables F_{B_r} and $F_t^{\pm}$ become compatibles and the auxiliary function (3.3) recover a proper probabilistic interpretation. Thus, in agreement with the conclusions in [21], we find that conditional time delays (i.e., asymptotic phase times) are the only well-defined (in the probabilistic sense) conditional time-statements in the context of the quantum scattering process.

6) The Larmor clock, originally introduced in [23],[24], is a concievable way of measuring directly the sojourn time by means of the precession of a spin in a weak magnetic field (see [25] and references therein). The Larmor clock has also been used to define transmission and reflection sojourn times by considering the spin precession associated with the transmitted and reflected waves separately. It is interesting to note that the times thus obtained (the so-called local Larmor times) are nothing but the transmission and reflection sojourn times (3.5) (see for instance [26]).

7) It is worth noting that the naive correspondance $X_t^{\pm} X_{B_r} \longleftrightarrow F_t^{\pm} F_{B_r}$ leads to the so-called complex interaction times which have received a formulation in terms of Feynman path-integrals [27]-[29] (in [29] the authors give the same negative conclusion about the possibility of obtaining a unique quantum definition for the duration of a tunneling event). The imaginary parts of these times, the so-called Büttiker Larmor times [30], contain an information on the variation of transmission and reflection probabilities with respect to energy and in the context of the Larmor clock method they are related to the change of the spin component parallel to the field direction when transmitted and reflected particles are considered separately.

4. Three-dimensional quantum scattering

We consider in this section a (one-body) potential scattering system in three dimensions. The Hilbert space is $\mathcal{H} \equiv L^2(\mathbb{R}^3)$ and the free hamiltonian is $H_0 = -\Delta/2m$ ($\hbar = 1$ and m is the mass of the particle) where Δ denotes the laplacian on $L^2(\mathbb{R}^3)$. The total hamiltonian is $H = H_0 + V$ where the potential V is assumed to be such that the wave operators exist, are complete and the scattering operator is unitary [16].

Let F be an arbitrary projection operator in $\mathcal{H}$. Then, according to the analysis of the preceeding sections, we define the time delay $\tau^F(\varphi)$ of the scattering process with incoming state φ and for a scattered state which is observed in the subspace $F\mathcal{H}$, as the limit

$$\tau^F(\varphi) \equiv \lim_{r \to \infty} \left(T^F(B_r, \varphi) - T^{0,F}_{out}(B_r, \varphi) \right) \tag{4.1}$$

where (see (3.5),(3.7))

$$T^F(B_r,\varphi) \equiv \mathrm{Re}\left(\frac{(\varphi, S^\dagger F S T_{B_r}\varphi)}{\| FS\varphi \|^2}\right), \quad T^{0,F}_{\mathrm{out}}(B_r,\varphi) \equiv \mathrm{Re}\left(\frac{(\varphi, S^\dagger F S (S^\dagger T^0_{B_r} S)\varphi)}{\| FS\varphi \|^2}\right). \tag{4.2}$$

For simplicity, we shall study the limit (4.1) in the simple case of a finite-range spherically symmetric potential ($R > 0$, $V(r) = 0$ if $r \geq R$) and for an incoming state φ belonging to the dense set of states of Schwartz functions with compact support on the spectrum of H_0 and having a finite number of components in the basis $|\ell, m)$ of eigenvectors of the orbital momentum. Then, the sojourn time $T_{B_r}(E)$, at energy E, admits the following decomposition

$$T_{B_r}(E) = \sum_{\substack{\ell=0 \\ |m|\leq\ell}}^{\infty} |\ell,m) T^\ell_{B_r}(E) (\ell,m| \tag{4.3}$$

where, for $r \geq R$ (see for instance [1]),

$$T^\ell_{B_r}(E) = \frac{2rm}{\sqrt{2mE}} - iS^*_\ell(E)\frac{dS_\ell(E)}{dE} - \frac{1}{2E}\sin(2\sqrt{2mE}r - \ell\pi + 2\delta_\ell(E)) \tag{4.4}$$

and $\delta_\ell(E)$ is the phase shift for the energy E and the angular momentum ℓ i.e., $S_\ell(E) \equiv (\ell,m|S(E)|\ell,m) = \exp(2i\delta_\ell(E))$. For the free sojourn time we have obviously the same expression with

$$\begin{aligned} T^{0,\ell}_{B_r}(E) &\equiv (\ell,m|T^0_r(E)|\ell,m) = (\ell,m|S^\dagger(E)T^0_r(E)S(E)|\ell,m) \\ &= \frac{2rm}{\sqrt{2mE}} - \frac{1}{2E}\sin(2\sqrt{2mE}r - \ell\pi). \end{aligned} \tag{4.5}$$

We shall now assume that the projection operator F is, in momentum space, multiplication by a function of the angles only. Then, the difference $T^\ell_{B_r}(E) - T^{0,\ell}_{B_r}(E)$ is to be averaged between the smooth wave packets $\varphi_{\ell,m}(E)$ and $(S^\dagger FS\varphi)_{\ell,m}(E)$ and thus converges weakly, as $r \to \infty$, to $-iS^*_\ell(E)dS_\ell(E)/dE = 2d\delta_\ell(E)/dE$ since the oscillating terms in (4.4) and (4.5) do not contribute because of the Riemann-Lebesgue lemma. Finally, using $SS^\dagger = I$ (or equivalently $S_\ell(E)S^*_\ell(E) = 1$), we obtain for the conditional time delay the formula

$$\tau^F(\varphi) = \mathrm{Re}\left(\frac{(\varphi, S^\dagger F(-idS/dH_0)\varphi)}{\| FS\varphi \|^2}\right). \tag{4.6}$$

The proof of the existence of the limit (4.1) and its identity to the formula (4.6) could be extended to the case of more general potentials (not necessarily spherically symmetrics) for a suitable class of initial states φ, by the time-dependent methods of [6]. Formula (4.6) is the natural generalization of the Eisenbud-Wigner formula (1.5),(1.6) which is simply recovered by setting $F = I$. It also constitute, as we shall see, the natural generalization of the angular time delay formula (1.7). For this, let F be the projection operator onto the

subspace of states the momentum of which lies in the cone $C(\hat{k}_2,\alpha) \equiv \{\vec{k} \in \mathbf{R}^3 | \vec{k}\cdot\hat{k}_2 \geq \alpha|\vec{k}|\}$ ($|\hat{k}_2| = 1$ and $0 < \alpha \leq 1$) and let $\Omega(\hat{k}_2,\alpha)$ be the part of the surface of the unit sphere $S^{(2)}$ lying in the cone $C(\hat{k}_2,\alpha)$. Clearly $F = \int_{\Omega(\hat{k}_2,\alpha)} d^2k\, |\hat{k})(\hat{k}|$. To derive the angular time delay formula (1.7) from (4.6) we need to make the two following assumptions:

(i) the modulus of the incoming wave packet φ is sharply peacked in momentum space about $\vec{k}_1 = \sqrt{2mE}\hat{k}_1$;

(ii) relative to this sharp peack the S-matrix and its energy derivative are slowly varying functions with respect to all variables (energy and angles).

Then, we have the approximations

$$(S\varphi)(E,\hat{k}) = \int_{S^{(2)}} d^2k'\, (\hat{k}|S(E)|\hat{k}')\varphi(E,\hat{k}') \approx A(E)(\hat{k}|S(E)|\hat{k}_1) \tag{4.7}$$

where $A(E) \equiv \int_{S^{(2)}} d^2k'\, \varphi(E,\hat{k}')$. Thus, we obtain

$$\begin{aligned} \| FS\varphi \|^2 &= \int_0^\infty dE' \int_{\Omega(\hat{k}_2,\alpha)} d^2k\, |(S\varphi)(E',\hat{k})|^2 \approx \int_0^\infty dE' \int_{\Omega(\hat{k}_2,\alpha)} d^2k\, |A(E')|^2 |(\hat{k}|S(E')|\hat{k}_1)|^2 \\ &\approx \int_0^\infty dE'\, |A(E')|^2 \int_{\Omega(\hat{k}_2,\alpha)} d^2k\, |(\hat{k}|S(E)|\hat{k}_1)|^2 \end{aligned} \tag{4.8}$$

and in an analogous way one finds

$$(\varphi, S^\dagger F(-idS/dH_0)\varphi) \approx \int_0^\infty dE'\, |A(E')|^2 \int_{\Omega(\hat{k}_2,\alpha)} d^2k\, (\hat{k}_1|S^\dagger(E)|\hat{k})(\hat{k}| - idS(E)/dE|\hat{k}_1). \tag{4.9}$$

Finally, inserting (4.8) and (4.9) into (4.6) and taking the limit $\alpha \to 1$, we obtain

$$\tau^F(\varphi) \approx \mathrm{Re}\left(-i\frac{(\hat{k}_2|dS(E)/dE|\hat{k}_1)}{(\hat{k}_2|S(E)|\hat{k}_1)}\right) = \frac{d}{dE}\arg(\hat{k}_2|S(E)|\hat{k}_1) \tag{4.10}$$

which is the desired angular time delay formula (1.7).

To conclude, consider the case where F is the projection operator onto the one-dimensional subspace generated by a (sufficiently smooth in energy) state ξ i.e., $F = |\xi)(\xi|$. Then, we come down to a notion of state-to-state time delay i.e., the time delay associated to the transition $\varphi \to \xi$. We have the formula

$$\tau^F(\varphi) = \mathrm{Re}\left(-i\frac{(\xi,(dS/dH_0)\varphi)}{(\xi,S\varphi)}\right). \tag{4.11}$$

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Appendix A

In this appendix we derive explicit expressions for the transmission and reflection time delays (2.21). We shall do it in some details only for the transmitted case. Let $(x_-(t),p_-(t)) \equiv \Phi_t \circ \Omega_-(x_0,p_0)$, we have

$$\begin{aligned} T^+(B_r,f) &= \int_{-\infty}^{\infty} dt\, P_t(B_r|+,\varphi) \\ &= P^+(\varphi)^{-1} \int_{-\infty}^{\infty} dt \int_{-\infty}^{\infty} dx \int_{-\infty}^{\infty} dp\, X_t^+(x,p) X_{B_r}(x,p) f_t(x,p) \\ &= P^+(\varphi)^{-1} \int_{-\infty}^{\infty} dt \int_{-\infty}^{\infty} dx_0 \int_{-\infty}^{\infty} dp_0\, X_{B_r}(x_-(t),p_-(t)) f^+(x_0,p_0) \\ &= P^+(\varphi)^{-1} \int_{-\infty}^{\infty} dt \int_{-\infty}^{\infty} dx_0 \int_{-\infty}^{\infty} dp_0 \int_{-r}^{r} dy\, \delta(y - x_-(t)) f^+(x_0,p_0) \end{aligned} \tag{A.1}$$

where for the third equality we have made the change of variables $(x,p) = \Phi_t \circ \Omega_-(x_0,p_0)$ and δ is the Dirac delta-function. At this step we note that for a transmitted trajectory

$$p_-(t) = \sqrt{p_0^2 - 2mV(x_-(t))}. \tag{A.2}$$

Thus, making the change of variable $z = x_-(t), dt = (m/\sqrt{p_0^2 - 2mV(z)})dz$ and integrating with respect to z, we obtain

$$\begin{aligned} T^+(B_r,f) &= P^+(\varphi)^{-1} \int_{-\infty}^{\infty} dx_0 \int_0^{\infty} dp_0 \int_{-r}^{r} dy\, \frac{m}{\sqrt{p_0^2 - 2mV(y)}} f^+(x_0,p_0) \\ &= P^+(\varphi)^{-1} \int_{-\infty}^{\infty} dx_0 \int_0^{\infty} dp_0 \left[\int_{-\infty}^{\infty} dy \left(\frac{m}{\sqrt{p_0^2 - 2mV(y)}} - \frac{m}{\sqrt{p_0^2}} \right) + \frac{2rm}{p_0} \right] f^+(x_0,p_0) \end{aligned} \tag{A.3}$$

where for the second equality we have used the fact that $(-r,r)$ contains the finite range of the potential. Let $f^{\pm}(E) \equiv \sqrt{\frac{m}{2E}} \int_{-\infty}^{\infty} dx_0 f^{\pm}(x_0, \sqrt{2mE})$ and

$$\alpha_{\rm cl}^+(E) \equiv \int_{-\infty}^{\infty} dy \left(\sqrt{2m(E - V(y))} - \sqrt{2mE} \right). \tag{A.4}$$

Then, (A.3) may be rewritten into the form

$$T^+(B_r,f) = P^+(\varphi)^{-1} \int_0^{\infty} dE\, f^+(E) \left(\frac{d\alpha_{\rm cl}^+(E)}{dE} + \frac{2rm}{\sqrt{2mE}} \right). \tag{A.5}$$

In an analogous way one can easily show that

$$T^{-}(B_r,f)=P^{-}(\varphi)^{-1}\int_0^{\infty}dE\,f^{-}(E)\left(\frac{d\alpha_{\rm cl}^{-}(E)}{dE}+\frac{2rm}{\sqrt{2mE}}\right) \tag{A.6}$$

where

$$\alpha_{\rm cl}^{-}(E)\equiv 2\int_{-\infty}^{\tilde{x}(E)}dy\,\left(\sqrt{2m(E-V(y))}-\sqrt{2mE}\right)+2\tilde{x}(E)\sqrt{2mE}, \tag{A.7}$$

$\tilde{x}(E)\equiv\inf_x\{x|E-V(x)=0\}$ is the reflection point for an incoming particle with energy E and we have assumed $\tilde{x}(E)\leq 0$ for all E. For the free reference times one finds

$$T_{\rm out}^{0,\pm}(B_r,f)=P^{\pm}(\varphi)^{-1}\int_0^{\infty}dE\,f^{\pm}(E)\frac{2rm}{\sqrt{2mE}}. \tag{A.8}$$

Finally, using (A.5),(A.6) and (A.8) into (2.21) we obtain (2.23).

Notice that since transmission occurs if $E-\sup_x V(x)>0$ (and conversely for reflection) one simply has

$$f^{\pm}(E)=\Theta\left(\pm(E-\sup_x V(x))\right)f(E) \tag{A.9}$$

where $f(E)\equiv\sqrt{\frac{m}{2E}}\int_{-\infty}^{\infty}dx_0 f(x_0,\sqrt{2mE})$.

Appendix B

In this appendix we indicate how to derive explicit expressions for the transmission and reflection time delays (3.8). For this, it is convenient to work in the two valued energy representation specified by $E=k^2/2m$ and $k/|k|$. The scattering operator on the energy shell $S(E)$ is then given by a 2×2 unitary matrix with elements $(\rho|S(E)|\sigma)$, $\rho,\sigma\in\{+,-\}$ where $(+|S(E)|+)=(-|S(E)|-)$ is the transmission coefficient at energy E and $(-|S(E)|+),(+|S(E)|-)$ are respectively the reflection coefficients for a particle coming from the left and from the right. The sojourn time operator $T_{B_r}(E)$ on the energy shell is also a 2×2 matrix with elements

$$(\rho|T_{B_r}(E)|\sigma)=\frac{m}{\sqrt{2mE}}\int_{-r}^{r}dx\,\psi_\rho^*(E,x)\psi_\sigma(E,x),\quad \rho,\sigma\in\{+,-\} \tag{B.1}$$

where $\psi_\pm(E,x)=\sqrt{2\pi}(2E/m)^{1/4}\langle x|\Omega_-|E,\pm\rangle$ are the solutions of the stationary Schrödinger equation $H\psi_\pm(E,x)=E\psi_\pm(E,x)$, with asymptotic forms

$$\begin{aligned}\psi_+(E,x)&=e^{i\sqrt{2mE}x}+(-|S(E)|+)e^{-i\sqrt{2mE}x}\qquad x\leq x_1\\ \psi_+(E,x)&=(+|S(E)|+)e^{i\sqrt{2mE}x}\qquad x\geq x_2\end{aligned} \tag{B.2}$$

and

$$\begin{aligned}\psi_-(E,x)&=(-|S(E)|-)e^{-i\sqrt{2mE}x}\qquad x\leq x_1\\ \psi_-(E,x)&=e^{-i\sqrt{2mE}x}+(+|S(E)|-)e^{i\sqrt{2mE}x}\qquad x\geq x_2.\end{aligned} \tag{B.3}$$

Observing that $\psi^*_\rho(E,x)\psi_\sigma(E,x) = \frac{1}{2m}\partial h_{\rho,\sigma}(E,x)/\partial x$ where

$$h_{\rho,\sigma}(E,x) = \left(\frac{\partial\psi^*_\rho}{\partial x}\frac{\partial\psi_\sigma}{\partial E} - \psi^*_\rho\frac{\partial^2\psi_\sigma}{\partial x\partial E}\right)(E,x) \tag{B.4}$$

one can use (B.2),(B.3) and (B.4) to derive explicit expressions for the matrix elements (B.1), when the interval $(-r,r)$ contains the range of the potential (in our case $(-r,r) \supset (x_1,x_2)$). Let φ be a sufficiently well behaved incoming state describing a particle approaching the potential barrier from the left i.e., $(P\varphi)(E) = \sqrt{2mE}\varphi(E)$ where $\varphi(E)$ is, for example, a Schwartz function with compact support and no support in a neighbourhood of the origin. Then, an explicit calculation yields

$$T^\pm(B_r,\varphi) = P^\pm(\varphi)^{-1}\int_0^\infty dE\,|A^\pm(E)\varphi(E)|^2\left(\frac{d\alpha^\pm(E)}{dE} + \frac{2rm}{\sqrt{2mE}} + A^\pm_{\text{int}}(E,r)\right) \tag{B.5}$$

where $A^\pm(E) = |A^\pm(E)|\exp(i\alpha^\pm(E)) \equiv (\pm|S(E))|+)$ and the interference terms $A^\pm_{\text{int}}(E,r)$ are given by

$$\begin{aligned} A^+_{\text{int}}(E,r) &= \frac{|A^-(E)|}{2E}\sin(\alpha^-(E)-\alpha^+(E))\cos(\alpha^+(E)+2\sqrt{2mE}r) \\ A^-_{\text{int}}(E,r) &= A^+_{\text{int}}(E) + \frac{1}{2E|A^-(E)|}\cos(\alpha^-(E)-\alpha^+(E))\sin(\alpha^+(E)+2\sqrt{2mE}r). \end{aligned} \tag{B.6}$$

Moreover, one obtains for the free reference times

$$T^{0,\pm}_{\text{out}}(B_r,\varphi) = P^\pm(\varphi)^{-1}\int_0^\infty dE\,|A^\pm(E)\varphi(E)|^2\left(\frac{2rm}{\sqrt{2mE}} + A^{0,\pm}_{\text{int}}(E,r)\right) \tag{B.7}$$

where $A^{0,+}_{\text{int}}(E,r) = 0$ and $A^{0,-}_{\text{int}}(E,r) = \sin(2\sqrt{2mE}r)/2E|A^-(E)|$. Finally, inserting (B.5) and (B.7) into (3.8) and noting that the oscillating interference terms do not contribute because of the Riemann-Lebesgue lemma, we find (3.10).

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