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Dwell times for light and electrons

Bart A van Tiggelen†, Adriaan Tip† and Ad Lagendijk†‡

† FOM-Institute for Atomic and Molecular Physics, Kruislaan 407, 1098 SJ Amsterdam, The Netherlands

‡ Van der Waals–Zeeman Laboratory, University of Amsterdam, Valckenierstraat 65–67, 1018 XE Amsterdam, The Netherlands

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Abstract. Using a time-dependent scattering theory for light we obtain expressions for the time that light spends in a finite dielectric medium surrounded by vacuum, the so-called dwell time. Given an incoming wavepacket, we focus upon the light scattered in an arbitrary direction. In view of the similarity between Maxwell's equations and the Schrödinger equation, some useful results are derived for the case of Schrödinger potential scattering as well. We show that the dwell time of a Schrödinger particle is a derivative of the phase shifts with respect to the potential, rather than to energy as is the case for the phase-delay time. We indicate the relation to absorption arguments. Because the potential for classical waves is energy dependent, derivatives of the phase shift with respect to potential enter into the phase-delay time for classical waves.

1. Introduction

The *dwell time* was first introduced by Smith [1] in the context of collision theory, and is sometimes also referred to as *sojourn time* [2] or *mean time* [3]. It is a concept that provides a measure of the time that some specified wavepacket 'spends' in some area in coordinate space. The nature of the wave can be either quantum mechanical or classical. The first case often addresses electrons in potentials, in the latter case one can think of acoustic or electromagnetic waves.

The introduction of the *time delay* by Wigner [4,5], was the first attempt to estimate how long a quantum-mechanical wavepacket is delayed by a scattering obstacle. The *phase-delay time* is expressed as a derivative of the phase shift ϕ of the scattering matrix with respect to energy,

$$\tau_p(E) = \frac{d\phi(E)}{dE}. \quad (1)$$

Later, Jauch *et al* [3] published an alternative but equivalent definition of time delay, namely

$$\tau_p[\psi^0] = \lim_{a \rightarrow \infty} \int_{-\infty}^{\infty} dt [\langle \psi_t | \chi_a | \psi_t \rangle - \langle \psi_t^0 | \chi_a | \psi_t^0 \rangle]. \quad (2)$$

In this formula $|\psi_t\rangle$ represents the (normalized) quantum mechanical wavefunction at time t and $|\psi_t^0\rangle$ is the unperturbed incoming wavepacket; χ_a is an operator projecting

onto a sphere of radius a in coordinate space. A subtraction of the incoming wave is not only physically plausible as a probe of time delay, it also guarantees that the limit $a \rightarrow \infty$ is finite. It was shown by both Jauch *et al* [3] and Martin [6] that this definition of time delay is, in essence, consistent with the phase-delay time put forward by Wigner.

Equation (2) suggests the definition of the following time:

$$\tau_C[\psi^0] = \int_{-\infty}^{\infty} dt \langle \psi_t | \chi_C | \psi_t \rangle \quad (3)$$

where C is some finite region in coordinate space. This time is anticipated to be finite if the wavefunction finally leaves the region C . This is typically true when the time-evolution operator has an absolute continuous spectrum. Following Martin [6], Büttiker [7] and other workers we will refer to this time as the *dwelt time* of C . The phase-delay time is readily expressed as the difference between the dwell time of the perturbed and unperturbed wavefunction for a very large region C .

If this region C is the region B in which the potential is non-zero (and is assumed to be bounded for simplicity), the dwell time τ_B should provide information about how long the wavepacket has spent inside the potential region. Especially near resonances the wave is trapped only inside B , and is essentially free outside. Consequently, any delay is expected to be contained in both the dwell time τ_B and in the phase-delay time τ_p . The similarity between both times also becomes apparent by the notion (as will be shown in this paper) that the dwell time τ_B for Schrödinger particles, as defined in equation (3), is in fact a derivative of the same phase shift of equation (1) with respect to the potential, rather than energy. On the level of t -matrices, we demonstrate that a small imaginary part of the potential (resembling the presence of an additional stationary scattering channel) yields a very convenient expression for the dwell time.

Treating the Maxwell equations as a set of first-order differential equations, it will turn out that, apart from some extra bookkeeping, the procedure to define dwell times for light is similar to Schrödinger potential scattering. An important intrinsic difference from the Schrödinger equation, namely the presence of an energy-dependent potential, will be discussed in relation to the Jauch formula (2) and a recently discovered decrease in the speed of light in media containing randomly placed resonant dielectric scatterers [8,9]. The energy dependence of the potential causes derivatives with respect to potential to appear in the phase-delay time for classical waves.

The time-delay problem has recently been given renewed attention. It was realized that the phase-delay time is not capable of giving a reasonable estimate of the delay caused by a *tunnelling process*. The (monochromatic equivalent of the) phase-delay time in equation (1) is known to saturate in the extreme opaque limit, thereby giving rise to an (apparent) violation of Einstein causality. Some alternative 'characteristic times' have been put forward, among which the Landauer-Büttiker time [10] and the Larmor time [7] are the most important [11]. The latter is obtained by probing the spin precession of a (tunnelling) electron. In a recent paper Martin and Bianchi [12] demonstrated very elegantly that the (asymptotic) Larmor time and the phase-delay time, in fact, coincide. The Landauer-Büttiker time, on the other hand, emerges from considerations pertaining to an *oscillating barrier* [13]. It seems that the characteristic time proposed by Landauer and Büttiker could be referred to as an *interaction time*

and does not necessarily probe the time that a wavepacket is being delayed. Rather, it estimates the time of interaction with an additional *dynamical* degree of freedom. If this is true, it is not at all clear that different (proposed) experiments [14–16] actually deal with the same time.

In this paper we will not make any attempt to shine new light on the interaction time. Rather, the purpose of this paper is to arrive at general results for the dwell time. In the next section we discuss the situation of Schrödinger waves in one dimension. In section 3 we outline a time-dependent theory for light scattering. This theory is used in section 4 in order to deal with the dwell time of light in three dimensions. We will focus upon the concept of *conditional dwell time*. This is the dwell time of a specified part of the wavepacket, for instance the part that finally emerges in some small solid angle. In section 5 we derive a ‘Jauch formula’ of the kind (2) for scalar waves.

2. Dwell times for 1D Schrödinger particles

The Schrödinger equation in one dimension is the simplest equation that mimics most relevant physics with respect to the dwell time. For this case, we will introduce the concept of *conditional dwell time*, in order allow for a comparison to the Maxwell situation.

Given a time-dependent solution $|\psi_t\rangle$ of the Schrödinger equation, the dwell time has already been defined in equation (3). The projection operators P_{\pm} are defined according to

$$\langle p|P_{\pm}|\psi\rangle = \theta(\pm p)\psi(p) \quad (4)$$

with associated eigenspaces \mathcal{H}_{\pm} ; the function $\theta(p)$ is the Heaviside step function. If we assume that the incoming wavepacket is originally in \mathcal{H}_+ , these eigenspaces correspond to the reflection (–) and transmission (+) channel. In terms of the S -matrix, the asymptotic solution of the Schrödinger equation is given by

$$|\psi_t\rangle = \begin{cases} t \rightarrow -\infty & \exp(-iH_0t)P_+|\psi^0\rangle \\ t \rightarrow +\infty & \exp(-iH_0t)SP_+|\psi^0\rangle. \end{cases} \quad (5)$$

The asymptotic reflected and transmitted part of the wavefunction are obtained by projecting the solution at $t \rightarrow \infty$ onto the corresponding eigenspace. Translating back to finite times we arrive at

$$|\psi_T(t)\rangle = \Omega_+ \exp(-iH_0t)S_{++}|\psi^0\rangle \quad (6)$$

$$|\psi_R(t)\rangle = \Omega_+ \exp(-iH_0t)S_{-+}|\psi^0\rangle. \quad (7)$$

For brevity $S_{++} \equiv P_+SP_+$, $S_{-+} \equiv P_-SP_+$. In terms of the Møller wave operators,

$$\Omega_{\pm} = \lim_{t \rightarrow \pm\infty} \exp(iHt) \exp(-iH_0t) \quad (8)$$

the S -matrix is given by $S = \Omega_+^* \Omega_-$. We can define the *transmission* and *reflection* time as

$$\tau_{T,R}(C) \equiv \int_{-\infty}^{\infty} dt \frac{\langle \psi_{T,R}(t) | \chi_C | \psi_{T,R}(t) \rangle}{\langle \psi_{T,R} | \psi_{T,R} \rangle}. \quad (9)$$

C is an as yet unspecified bounded region in coordinate space with projector χ_C . The integrand of equation (9) is interpreted as the probability of finding the particle in C at time t , provided it finally emerges in either the transmission or reflection channel. As such, we shall refer to the times τ_T and τ_R as conditional dwell times for both channels. Recently, a similar conditional variant of the phase-delay time was presented in [17].

The definition in equation (9) can be worked out formally by insertion of the set $\{|p\rangle\}$, satisfying $H_0|p\rangle = p^2|p\rangle$, and

$$\sum_p |p\rangle\langle p| = 1 \quad \langle p'|p\rangle = 2\pi\delta(p-p') \quad (10)$$

where $\sum_p \equiv \int dp/2\pi$. The S -matrix takes the form

$$\langle p'|S|p\rangle = 2\pi\delta(p-p')T_p + 2\pi\delta(p+p')R_p \quad (11)$$

R_p and T_p are the complex reflection and transmission coefficients at energy $E = p^2$. The unitarity of S gives rise to

$$|T_p|^2 + |R_p|^2 = 1 \quad T_p^* R_{-p} + R_p^* T_{-p} = 0. \quad (12)$$

It can be checked that

$$\langle p|S_{++}|\psi^0\rangle = \theta(p)T_p\psi^0(p) \quad \langle p|S_{-+}|\psi^0\rangle = \theta(-p)T_{-p}\psi^0(-p). \quad (13)$$

The numerator of the transmission time can be worked out to

$$\int_{-\infty}^{\infty} dt \sum_{pp'} \langle \psi^0|S_{++}^*|p\rangle e^{-ip^2t} \langle p|\Omega_{\pm}^* \chi_C \Omega_{\pm}|p'\rangle e^{ip'^2t} \langle p'|S_{++}|\psi^0\rangle.$$

The time integral yields a factor $2\pi\delta(p^2-p'^2)$ and brings the conditional dwell times on the energy shell. We define the matrix element

$$W_{pp'}(C) = \langle p|\Omega_{\pm}^* \chi_C \Omega_{\pm}|p'\rangle \equiv \langle \varphi^-(p)|\chi_C|\varphi^-(p')\rangle. \quad (14)$$

Since $\Omega_{\pm} H_0 = H \Omega_{\pm}$ it formally follows that $|\varphi^{\mp}(p)\rangle \equiv \Omega_{\pm}|p\rangle$ is a continuum eigenfunction of H at eigenvalue p^2 , which (again formally) satisfies, by the isometry of the wave operators, continuum normalization. This set of eigenfunctions is usually referred to as distorted incoming ($-$) or outgoing ($+$) plane waves. The proper justification for these formal manipulations requires results from the theory of 'generalized eigenfunction' expansion of Schrödinger operators [18].

The transmission time now becomes identical to

$$\tau_T(C) = \frac{\int_0^{\infty} dp (2p)^{-1} W_{pp}(C) |T_p|^2 |\psi^0(p)|^2}{\int_0^{\infty} dp |T_p|^2 |\psi^0(p)|^2}. \quad (15)$$

Similarly, we obtain for the reflection time,

$$\tau_R(C) = \frac{\int_0^{\infty} dp (2p)^{-1} W_{-p,-p}(C) |R_p|^2 |\psi^0(p)|^2}{\int_0^{\infty} dp |R_p|^2 |\psi^0(p)|^2}. \quad (16)$$

The total dwell time (without projections upon any outgoing channel) is

$$\tau_d(C) = \int_0^\infty \frac{dp}{2p} [W_{pp}(C)|T_p|^2 + W_{-p,-p}(C)|R_p|^2 + 2\text{Re}(W_{p,-p}(C)T_p^*R_p)]|\psi^0(p)|^2. \quad (17)$$

The third term amounts to an interference between the reflecting and transmitting part of the wavefunction inside the region C . From now on we shall take C to be equal to the support B of the potential. Before we proceed, we note that

$$\langle \varphi^+(p) | \chi_B | \varphi^+(p') \rangle = \langle \varphi^-(-p') | \chi_B | \varphi^-(-p) \rangle \quad (18)$$

$$T_p = T_{-p}. \quad (19)$$

These identities follow from the time-reversal symmetry of the Schrödinger wave equation. The following formulae relate the matrix element $W_{pp'}(B)$ to the transmission and reflection coefficients,

$$W_{-p',-p}(B) = i \frac{R_p^* - R_{p'}}{p + p'} + i \frac{R_p^* R_{p'} + T_p^* T_{p'} e^{i(p+p')d} - 1}{p - p'} \quad (20a)$$

$$W_{+p',-p}(B) = i \frac{T_p^* e^{-i(p'+p)d} - T_{-p'}}{p + p'} + i \frac{R_p^* T_{-p'} + R_{-p'} T_p^* e^{-i(p-p')d}}{p - p'}. \quad (20b)$$

We have taken $B = [0, d]$ and $p, p' > 0$. The derivation runs as follows. For $p > 0$,

$$\langle r | \varphi^+(p) \rangle = \begin{cases} e^{ipr} + R_p e^{-ipr} & r < 0 \\ B_p(r) & 0 < r < d \\ T_p e^{ipr} & r > d. \end{cases} \quad (21)$$

Since

$$\langle \varphi^+(p) | \varphi^+(p') \rangle = 2\pi \delta(p - p') \quad W_{-p',-p}(B) = \int_0^d dr B_p^*(r) B_{p'}(r) \quad (22)$$

(20a) follows by simple integration, thereby applying equation (18). If $p < 0$,

$$\langle r | \varphi^+(p) \rangle = \begin{cases} e^{ipr} + R_p e^{-ipr} & r > d \\ B_p(r) & 0 < r < d \\ T_p e^{ipr} & r < 0. \end{cases} \quad (23)$$

and (20b) follows similarly.

The phase shifts $\phi_T(p)$ and $\phi_R(p)$ are defined according to $T_p = |T_p| \exp(i\phi_T)$, $R_p = |R_p| \exp(i\phi_R)$. In what follows, we focus on *inversion symmetric* (IS) potentials: $V(r) = V(d - r)$ [19]. One can check that inversion symmetry implies

$$R_p = R_{-p} e^{2ipd} \quad W_{pp'}(B) = W_{-p,-p'}(B) e^{i(p'-p)d} \quad (24)$$

From the reciprocity relation (12) one infers immediately that

$$\text{Re } T_p^* R_p e^{-ipd} = 0 \tag{25}$$

so that $\phi_R = \phi_T + pd \pmod{\pi}$. Hence,

$$\frac{d\phi_R}{dp} = \frac{d\phi_T}{dp} + d \equiv \frac{d\phi}{dp}. \tag{26}$$

From equation (20) the following results for inversion symmetric potentials can be obtained straightforwardly,

$$W_{pp}(B) = \frac{\text{Im } R_p}{p} + \frac{d\phi}{dp}. \tag{27a}$$

$$W_{p,-p}(B) = \frac{\text{Im}(T_p e^{ipd})}{p} e^{-ipd} + iR_p^* T_p \left(\frac{d \log |R_p|}{dp} - \frac{d \log |T_p|}{dp} \right) \tag{27b}$$

Near resonances $d\phi/dp$ is large and the dwell time of the potential region (being equal to $W_{pp}(B)/2p$) and the phase-delay time $d\phi/dp^2$ are approximately equal. The additional term in (27a) is caused by self-interference *outside* the potential region [11], where the wave would have been classically free. By using proposition (27a) an eigenfunction analogy of the Jauch formula (2) can be obtained. With $B_a = [-a, a]$,

$$\lim_{a \rightarrow \infty} [W_{pp}(B_a) - W_{pp}^0(B_a)] = |R_p|^2 \frac{d\phi_R}{dp} + |T_p|^2 \frac{d\phi_T}{dp} \stackrel{\text{IS}}{=} \frac{d\phi}{dp} - d|T_p|^2. \tag{28}$$

We give a formal proof of equation (28). Apart from $W_{pp}(B_a)$ in equation (20) the Jauch formula contains the free contribution W_{pp}^0 and the integral outside the barrier. Together this amounts to

$$\begin{aligned} & \int_{-a}^0 dr |e^{ipr} + R_p e^{-ipr}|^2 + \int_d^a dr |T_p e^{ipr}|^2 - \int_{-a}^a dr |e^{ipr}|^2 \\ &= 2 \text{Re } R_p^* \left(\frac{1 - e^{2ipa}}{2ip} \right) - d|T_p|^2 \stackrel{a \rightarrow \infty}{=} -\frac{\text{Im } R_p}{p} - d|T_p|^2. \end{aligned}$$

Using equation (27) this adds up to the result in equation (28). The exponent $\exp(2ipa)$ vanishes in the weak sense.

In the context of the Jauch formula, we mention that a similar formula can be derived for the matrix element $W_{p,-p}$. Restricting again to the case of inversion symmetry, it follows from equation (27) that

$$\lim_{a \rightarrow \infty} R_p T_p^* W_{p,-p}(B_a) = |T_p|^2 |R_p|^2 \left(d + i \frac{d \log |R_p|}{dp} - i \frac{d \log |T_p|}{dp} \right). \tag{29}$$

The free contribution $W_{p,-p}^0([-\infty, \infty]) = 0$. We remark that equation (27b) together with equation (25), implies that $R_p T_p^* W_{p,-p}(B)$ is purely imaginary. This means that the interference term in the total dwell time equation (17) vanishes. Hence,

$$\tau_d(B) = \int_0^\infty \frac{dp}{2p} W_{pp}(B) |\psi^0(p)|^2. \tag{30}$$

In the plane-wave limit we let $|\psi^0(p)|^2 \rightarrow \delta(p-k)$. For IS potentials one thus obtains

$$\tau_d(B, k) = \tau_R(B, k) = \tau_T(B, k) = \frac{1}{2k} W_{kk}(B). \quad (31)$$

We conclude that the 'transmission time', the 'reflection time' and the 'unconditional dwell time' coincide in the plane-wave limit for IS potentials. Because this time is expressed in terms of the matrix element $W_{kk}(B)$, we expect that knowledge of the matrix element $W_{k,-k}(B)$ reveals extra information about the potential. This is an interesting observation since the term between parentheses in equation (29) seems to be related to the complex-valued Landauer-Büttiker interaction time $\tau_{LB} \sim -\text{id}(\log T_p)/dp^2$ [13]. We will not deal with this issue any further.

In the appendix we find another representation for $W_{kk}(B)$, as well as a generalization to three dimensions. There we show that

$$\frac{1}{2k} W_{kk}(B) = -|R_k|^2 \delta_V^{\chi_B} \phi_R - |T_k|^2 \delta_V^{\chi_B} \phi_T = -\frac{1}{2} \delta_V^{\chi_B} [1 - |R_k|^2 - |T_k|^2]. \quad (32)$$

Here δ_V^ξ denotes a *functional derivative* with respect to the potential $V(r)$ in the direction $\xi(r)$. The characteristic function of the potential region B is again denoted by $\chi_B(r)$. The first equality is in complete agreement with equation (2.9) of [12]. The second equality is obtained by the introduction of a small imaginary part of the potential in the reflection and transmission coefficients. Such a procedure cannot, in general, be justified in time-dependent situations (see, however, Kato [20]), but here, on the level of transition matrices, there are no such problems. The outcome is very convenient for numerical computation.

Another useful result derived in the appendix is that if $V(r) = V_0 g(r)$ is the potential, then

$$\frac{1}{2k} \langle \varphi_k^+ | V | \varphi_k^+ \rangle = -|R_k|^2 V_0 \frac{\partial \phi_R}{\partial V_0} - |T_k|^2 V_0 \frac{\partial \phi_T}{\partial V_0} \stackrel{\text{IS}}{=} -V_0 \frac{\partial \phi}{\partial V_0}. \quad (33)$$

Only the rectangular potential (for which $g(r) = \chi_B(r)$) has the special property that derivatives of the phase shift with respect to V_0 equal the dwell time [7, 21]. We conclude that the dwell time of the potential region B is a derivative of the phase shifts with respect to the potential in the direction of the characteristic function of B . The phase-delay time, on the other hand, is a derivative of the same phase shifts with respect to energy. For Schrödinger potential scattering, both time scales coincide approximately near resonances [7].

3. Time-dependent scattering theory for light

The usual approach to dealing with Maxwell's equations is to eliminate either the magnetic or electric field component. In the absence of ohmic currents and magnetic interactions, this procedure gives the Helmholtz equation,

$$\nabla \times (\nabla \times \mathbf{E}) + \varepsilon(r) \partial_t^2 \mathbf{E} = 0 \quad (34)$$

in which $\varepsilon(r)$ is the dielectric permeability. The local speed of light is given by $c(r) = \varepsilon(r)^{-1/2}$. The Helmholtz equation bears a strong resemblance to the scalar wave equation:

$$-\nabla^2 \psi + \varepsilon(r) \partial_t^2 \psi = 0. \quad (35)$$

By the absence of polarization, the latter is much easier to deal with, especially in the case of multiple scattering. The scalar wave equation, in turn, is very similar to the Schrödinger equation,

$$-\nabla^2\psi + V(\mathbf{r})\psi = i\partial_t\psi. \quad (36)$$

By insertion of monochromatic waves, $\psi \sim \exp(-iEt)$, E playing the role of 'energy' in the quantum mechanical picture, and of 'frequency' in the scalar wave equation, it is seen that equations (35) and (36) are, in fact, identical, provided one identifies for scalar waves an energy $E^2 > 0$ and an *energy-dependent* potential

$$V(\mathbf{r}, E) = [1 - \varepsilon(\mathbf{r})]E^2. \quad (37)$$

For $\varepsilon(\mathbf{r}) > 1$ this potential is negative and thus attractive. In the presence of randomness in the dielectric constant $\varepsilon(\mathbf{r})$ this energy-dependency was recently shown to give a substantial renormalization of time scales in macroscopic (diffusive) transport of light, *not* present if similar randomness is imposed on the electron potential $V(\mathbf{r})$. The *stationary* properties of both equations, on the other hand, are equal in the sense that there is a one-to-one correspondence of (continuum) eigenfunctions.

To arrive at a time-dependent treatment of light scattering, the second-order time derivative is inappropriate, and the original Maxwell equations, being first order in time, are preferable to the Helmholtz equation. The framework of this theory was published recently by Dorren and one of us [22]. Equivalent time-dependent theories for classical waves are known from literature [23–25]. Therefore we will restrict ourselves to an overview of the most important results for our purposes.

We interpret $\varepsilon(\mathbf{r})$ as a positive, real-valued operator. With the operator $\Gamma = \varepsilon^{-1/2}$ and the six-dimensional state vector,

$$|\underline{\mathbf{E}}_t\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} \Gamma^{-1}|\mathbf{E}_t\rangle \\ |\mathbf{B}_t\rangle \end{pmatrix}. \quad (38)$$

the Maxwell equations take the convenient form,

$$i\partial_t|\underline{\mathbf{E}}_t\rangle = \underline{\mathbf{K}} \cdot |\underline{\mathbf{E}}_t\rangle. \quad (39)$$

The time-evolution generator $\underline{\mathbf{K}}$ is given by [22]

$$\underline{\mathbf{K}} = \begin{pmatrix} 0 & \Gamma(\boldsymbol{\varepsilon} \cdot \mathbf{p}) \\ -(\boldsymbol{\varepsilon} \cdot \mathbf{p})\Gamma & 0 \end{pmatrix}. \quad (40)$$

In this equation, $(\boldsymbol{\varepsilon} \cdot \mathbf{p})_{ij} = \sum_k \varepsilon_{ijk} p_k$ where ε_{ijk} is the Levi-Civita tensor density being anti-symmetric in all indices with the convention that $\varepsilon_{123} = 1$. This time evolution conserves transversality ($\nabla \cdot \mathbf{B}(t) = \nabla \cdot \mathbf{D}(t) = 0$), as well as the total electromagnetic energy,

$$W(t) = \frac{1}{2} \int d\mathbf{r} [\varepsilon(\mathbf{r})|\mathbf{E}(\mathbf{r}, t)|^2 + |\mathbf{B}(\mathbf{r}, t)|^2] \equiv \langle \underline{\mathbf{E}}_t | \underline{\mathbf{E}}_t \rangle. \quad (41)$$

We introduced the scalar product according to

$$\langle \underline{\mathbf{f}} | \underline{\mathbf{g}} \rangle = \int d\mathbf{r} \underline{\mathbf{f}}^*(\mathbf{r}) \cdot \underline{\mathbf{g}}(\mathbf{r}). \quad (42)$$

The associated Hilbert space is $\mathcal{K} = L^2(\mathbb{R}^3, d\mathbf{r}, \mathbb{C}^6)$, consisting of square-integrable six-dimensional vector fields on \mathbb{R}^3 . With respect to the inner product above, \underline{K} is a symmetric operator. The free time evolution \underline{K}_0 , obtained by setting $\Gamma = 1$, has an absolute continuous spectrum covering the whole real axis, and an imbedded eigenvalue zero corresponding to the longitudinal subspace \mathcal{K}_\perp in \mathcal{K} . The continuum transverse generalized eigenfunctions of \underline{K}_0 at the eigenvalue E are

$$|j\hat{k}, E\rangle \equiv \frac{1}{\sqrt{2}} \begin{pmatrix} g_j \\ \hat{k} \times g_j \end{pmatrix} |E\hat{k}\rangle \quad (E \in \mathbb{R}, j = \pm 1, \hat{k} \in 4\pi). \quad (43)$$

We observe a threefold degeneracy: two angles fixing the direction of propagation \hat{k} , and one index j representing two mutually orthogonal (normalized) choices for the polarization vector g . By transversality both these vectors must be perpendicular to the vector \hat{k} . The set of generalized eigenfunctions in equation (43) satisfies continuum normalization

$$\langle j\hat{k}, E | j'\hat{k}', E' \rangle = (2\pi)^3 \delta_{jj'} \delta(E - E') \delta(\hat{k} - \hat{k}') \quad (44)$$

$$\sum_{j\hat{k}E} |j\hat{k}, E\rangle \langle j\hat{k}, E| = \underline{\Pi}_0 \quad (45)$$

where $\underline{\Pi}_0 \equiv \Delta_p \underline{I}$ is the projector upon the transverse subspace \mathcal{K}^\perp in \mathcal{K} . We use the notation $\sum_{j\hat{k}E} = (2\pi)^{-3} \int dE \int d\hat{k} \sum_{j=\pm 1}$. As usual the Møller wave operators are defined as

$$\underline{\Omega}_\pm = s - \lim_{t \rightarrow \pm\infty} \exp(i\underline{K}t) \cdot \exp(-i\underline{K}_0t) \cdot \underline{\Pi}_0. \quad (46)$$

In terms of the wave operators, the scattering operator can be defined as $\underline{S} = \underline{\Omega}_+^* \cdot \underline{\Omega}_-$. When the wave operators exist and are complete, the S -matrix is on-shell, $\underline{S} \cdot \underline{K}_0 = \underline{K}_0 \cdot \underline{S}$, and unitary, $\underline{S}^* \cdot \underline{S} = \underline{S} \cdot \underline{S}^* = \underline{\Pi}_0$. It has the formal representation

$$\underline{S} = \underline{\Pi}_0 - 2\pi i \lim_{\epsilon \downarrow 0} \underline{\Pi}_0 \cdot \int \delta(E - \underline{K}_0) \cdot \underline{T}(E + i\epsilon) \cdot \underline{E}_0(dE) \quad (47)$$

where $\underline{E}_0(dE) = dE \sum_{i\hat{k}} |i\hat{k}, E\rangle \langle i\hat{k}, E|$. The transition operator is

$$\underline{T}(z) = \underline{V} + \underline{V} \cdot [z - \underline{K}]^{-1} \cdot \underline{V}. \quad (48)$$

For future use we construct the t -matrix or scattering amplitude $T_{jk_j'k'}(E^\pm)$,

$$T_{jk_j'k'}(E^\pm) = 2E \langle j\hat{k}, E | \underline{T}(E \pm i\epsilon) | j'\hat{k}', E \rangle. \quad (49)$$

Here $k = E\hat{k}$. A straightforward algebraic manipulation of the scattering amplitude, using the explicit form of the eigenstates $|j\hat{k}, E\rangle$ given in equation (43), yields for the scattering amplitude the convenient representation,

$$T_{jk_j'k'}(E^\pm) = \langle E\hat{k} | g_j^* \cdot T(E \pm i\epsilon) \cdot g_{j'} | E\hat{k}' \rangle \quad (50)$$

in which

$$T(z) = \Phi z^2 + \Phi z^2 \cdot [z^2 - p^2 \Delta_p - \Phi z^2]^{-1} \cdot \Phi z^2. \quad (51)$$

$T(z)$ is an operator working on three-dimensional vector fields. It has properties of a transition operator, corresponding to an energy-dependent, in general complex potential $\Phi z^2 = [1 - \epsilon(r)]z^2$ and complex energy z^2 . Indeed it can be viewed as the t -matrix of the Helmholtz equation (34). To our satisfaction, we observe that a time-evolution treatment of Maxwell's equations brings us back to the analogies with the Schrödinger wave equation mentioned at the beginning of this section.

4. Dwell times for light

The time-dependent scattering theory sketched above will now be applied to define and work out the dwell time in the Maxwell picture. Given a region B in coordinate space with projector χ_B , and an electromagnetic wavefunction $|\underline{E}_t\rangle$, the dimensionless quantity

$$\frac{W_B(t)}{W(t)} = \frac{\langle \underline{E}_t | \chi_B | \underline{E}_t \rangle}{\langle \underline{E}_t | \underline{E}_t \rangle} \quad (52)$$

is the relative amount of energy in region B at time t . We expect that $W_B(t) \rightarrow 0$ for $t \rightarrow \pm\infty$, because the wavepacket has either not yet reached or already left the region B . By energy conservation, the denominator in equation (52) does not depend on time. We can define the total dwell time as

$$\tau_B = \int_{-\infty}^{\infty} dt \frac{W_B(t)}{W}. \quad (53)$$

In terms of the S -matrix, the asymptotic solution of the scattering set-up, satisfying our constraints for both $t \rightarrow \pm\infty$ is

$$|\underline{E}_{t \rightarrow \infty}(i \rightarrow f)\rangle = \exp(-i\underline{K}_0 t) \cdot \underline{P}_f \cdot \underline{S} \cdot \underline{P}_i |\underline{E}^0\rangle.$$

Thus at finite times, as in section 2,

$$\begin{aligned} |\underline{E}_t(i \rightarrow f)\rangle &= \lim_{t' \rightarrow \infty} \exp(-i\underline{K}(t-t')) \cdot \exp(-i\underline{K}_0 t') \cdot \underline{P}_f \cdot \underline{S} \cdot \underline{P}_i |\underline{E}^0\rangle \\ &= \underline{\Omega}_+ \cdot \exp(-i\underline{K}_0 t) \cdot \underline{S}_{fi} |\underline{E}^0\rangle \end{aligned}$$

where equation (46) has been inserted for the wave operator. In addition $\underline{S}_{fi} = \underline{P}_f \cdot \underline{S} \cdot \underline{P}_i$. The *conditional dwell time* can now be defined according to

$$\tau_B(i \rightarrow f) \equiv \frac{D_B(i \rightarrow f)}{W(i \rightarrow f)} = \int_{-\infty}^{\infty} dt \frac{W_B(t, i \rightarrow f)}{W(i \rightarrow f)} \quad (54)$$

in which

$$\begin{aligned} W_B(t, i \rightarrow f) &= \langle \underline{E}_t(i \rightarrow f) | \underline{E}_t(i \rightarrow f) \rangle \\ &= \langle \underline{E}^0 | \underline{S}_{if}^* \cdot \exp(i\underline{K}_0 t) \cdot \underline{\Omega}_+^* \chi_B \underline{\Omega}_+ \cdot \exp(-i\underline{K}_0 t) \cdot \underline{S}_{fi} | \underline{E}^0 \rangle \end{aligned}$$

$$W(i \rightarrow f) = \langle \underline{E}^0 | \underline{S}_{if}^* \cdot \underline{S}_{fi} | \underline{E}^0 \rangle. \quad (55)$$

A similar approach holds for the Schrödinger wave equation in three dimensions. We can work out this expression by insertion of the plane-wave set equation (45). The numerator becomes

$$\begin{aligned} D_B(i \rightarrow f) &= \int_{-\infty}^{\infty} dt \sum_{n\hat{k}E} \sum_{n'\hat{k}'E'} e^{i(E-E')t} \\ &\quad \times \langle \underline{E}^0 | \underline{S}_{if}^* | n\hat{k}, E \rangle \langle n\hat{k}, E | \underline{\Omega}_+^* \chi_B \underline{\Omega}_+ | n'\hat{k}', E' \rangle \langle n'\hat{k}', E' | \underline{S}_{fi} | \underline{E}^0 \rangle. \quad (56) \end{aligned}$$

The time integral gives a factor $2\pi\delta(E - E')$. We construct the matrix element W in terms of the incoming distorted plane waves $|\varphi_{n\hat{k}}^-(E)\rangle$ mentioned earlier,

$$\langle\varphi_{n\hat{k}}^-(E)|\chi_B|\varphi_{n'\hat{k}'}^-(E)\rangle = W_{n\hat{k}n'\hat{k}'}(B, E). \quad (57)$$

The S -matrix in equation (47) can be sandwiched between the plane waves in equation (43) to give

$$\begin{aligned} \langle n\hat{k}, E|\underline{S}_{fi}|n'\hat{k}', E'\rangle \\ = \chi_f(n\hat{k})\chi_i(n'\hat{k}')\delta(E - E') \left[\delta_{nn'}\delta(\hat{k} - \hat{k}') - \frac{\pi i}{E} T_{nkn'\hat{k}'}(E^+) \right] \end{aligned} \quad (58)$$

where we have used the t -matrix $T_{nkn'\hat{k}'}(E^+)$ defined in section 3. Equation (56) now becomes

$$\begin{aligned} \frac{dD_B}{dE}(i \rightarrow f) = 2\pi \sum_{n\hat{k}} \sum_{n'\hat{k}'} \chi_i(n\hat{k})\chi_f(n'\hat{k}') W_{n\hat{k}n'\hat{k}'}(B, E) \\ \times [I_E^0(n'\hat{k}') - iI_E(n'\hat{k}')]^* [I_E^0(n\hat{k}) - iI_E(n\hat{k})]. \end{aligned} \quad (59)$$

We have written $I_E^0(n\hat{k}) = \langle n\hat{k}, E|\underline{F}^0\rangle$, and introduced the scattered amplitude in the channel $n\hat{k}$ as

$$I_E(n\hat{k}) = \frac{\pi}{E} \sum_{n''\hat{k}''} T_{nkn''\hat{k}''}(E^+) I_E^0(n''\hat{k}''). \quad (60)$$

For simplicity we have assumed that the incoming wavepacket satisfies our constraints, i.e. $|\underline{F}^0\rangle \in \underline{P}_i\mathcal{K}$. Equation (55) can now be written as

$$\frac{dW}{dE}(i \rightarrow f) = \sum_{n\hat{k}} [|I_E^0(n\hat{k})|^2 + |I_E(n\hat{k})|^2 + 2 \operatorname{Im}(I_E^0(n\hat{k})^* I_E(n\hat{k}))]. \quad (61)$$

This is recognized as the sum of a 'coherent' wave (i.e. propagating in the forward direction), a scattered part and the interference between them. Both in equation (59) and equation (61) we supposed that the initial wavepacket has support only in a small frequency range dE . Because the S -operator is on the energy shell, the asymptotic, scattered wave has the same support. The solution for a non-monochromatic wavepacket is recovered by integrating over frequencies E .

By combining equations (59) and (61) the conditional dwell time can be found. Starting from these general equations we can proceed by taking $\chi_i(n\hat{k}) = \delta_{ni}\theta(\hat{k} \in d\Omega_i)$ and $\chi_f(n\hat{k}) = \delta_{nm}\theta(\hat{k} \in d\Omega_f)$, thereby squeezing both the solid angles $d\Omega_i$ and $d\Omega_f$. Any small solid angle can be considered as a scattering channel. By definition, the *coherent channel* is the channel in which the forward propagating wave is present: $d\Omega_i = d\Omega_f$, $m = i$. A *scattering channel* is a channel in which there is no contribution from the forward propagating wave: $d\Omega_i \cap d\Omega_f = \emptyset$ or $j \neq i$. We get

$$\frac{d\tau_B}{d\Omega_i}(i\hat{p} \rightarrow i\hat{p}, E) = \frac{d\tau_B}{d\Omega_f}(j\hat{p}' \rightarrow i\hat{p}, E) = \left(\frac{E}{2\pi}\right)^2 W_{i\hat{p};i\hat{p}}(B, E). \quad (62)$$

We come to an unexpected property of the monochromatic limit: the conditional dwell time in a specific channel depends only on the orientation of the solid angle under consideration with respect to the dielectric scatterer B . The history, that is the channel through which the wavepacket originally entered, is completely forgotten! As in the Schrödinger situation, we infer that knowledge of the conditional dwell times requires information about the 'diagonal' matrix elements $W_{n\hat{k}n\hat{k}}(B)$ only. If the barrier has rotational symmetry, all channels, including the coherent channel, have the same conditional dwell time. This is no longer true beyond the monochromatic limit.

In the absence of symmetry, a dwell time averaged over outgoing channels can be constructed as

$$\frac{\tau_B(p)}{4\pi} \equiv \left(\frac{E}{2\pi}\right)^2 \langle W_{j\hat{p}'j\hat{p}'}(B, E) \rangle_{j\hat{p}'} = \frac{V_B}{\lambda^2} W(B, p). \quad (63)$$

We have introduced the wavelength $\lambda = 2\pi/E$, and the volume V_B of the region B ; $W(B, p)$ is identified as the averaged, normalized electromagnetic energy density in the region B (in a stationary situation).

Having found the (average) dwell time per scattering channel we discuss the following heuristic, but nevertheless very important *charging time*. In case the scattering region B is large compared to the wavelength λ , one can use the *ray concept* to visualize the scattering process. In this picture (figure 1) the incoming plane wave is considered as a collection of open input channels ('rays'), which have typical size $\lambda/2\pi$. If $\sigma(E)$ is the total scattering cross section, the number of open input channels is estimated as $\sigma(E)/\pi(\lambda/2\pi)^2 = 4\pi\sigma(E)/\lambda^2$. The average dwell time per open channel is called the charging time. By equation (63),

$$\tau_B^c(E) = \frac{V_B W(B, E)}{\sigma(E)}. \quad (64)$$

Since equation (64) takes into account the two-dimensional degeneracy of the incoming wave, the charging time rather than equation (63), is expected to give an estimate of the time spent by the light in the region B .

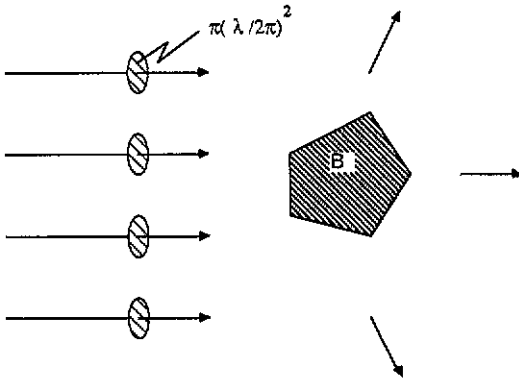


Figure 1. The ray picture for light scattering. The incoming plane wave is considered as a collection of input channels of 'extent' $\lambda/2\pi$ which can be either opened or closed. The number of open channels N is estimated using $N\pi(\lambda/2\pi)^2 = \sigma$.

The degeneracy problem can be handled rigorously for rotationally symmetric scatterers. In that case a partial wave analysis can be made, and a subsequent

projection of the scattered wave upon the subspace with specified 'rotational quantum numbers' n and l can be carried out. It is known [26] that for high frequencies such a partial wave treatment goes over into the ray concept mentioned above. To calculate $W(B, E)$ the eigenvalue problem has to be solved. For the *Mie sphere* the solution can be found in almost any text book on light propagation. The corresponding energy density for such sphere can then be calculated straightforwardly. The dwell time for a partial wave with principal quantum number n is, similarly to equation (63),

$$\tau_B^n(E) = \frac{4\pi}{\lambda^2} V_B W^n(B, E) \quad n = 1, 2, \dots \quad (65)$$

and does not depend on the magnetic quantum number. The energy density $W^n(B, p)$ is conveniently written in the form [27]

$$W^n(B, E) = \frac{3m}{4x^3} \lim_{m_i \rightarrow 0} \left(\frac{\operatorname{Re} a_n - |a_n|^2}{m_i} + \frac{\operatorname{Re} b_n - |b_n|^2}{m_i} \right) + \frac{3m}{4x^3} (|d_n|^2 - |c_n|^2) \psi_n(mx) \psi_n'(mx). \quad (66)$$

Here $x = Er_m$ is the size parameter, $\psi_n(x) \equiv x j_n(x)$; a_n and b_n are the standard (Van de Hulst) coefficients for the Mie sphere [26]. The parameters c_n and d_n , instead, characterize the electromagnetic field *inside* the sphere. In equation (66) a small absorption (or gain) $m_i \equiv \operatorname{Im} m$ has been introduced, similarly to equation (32).

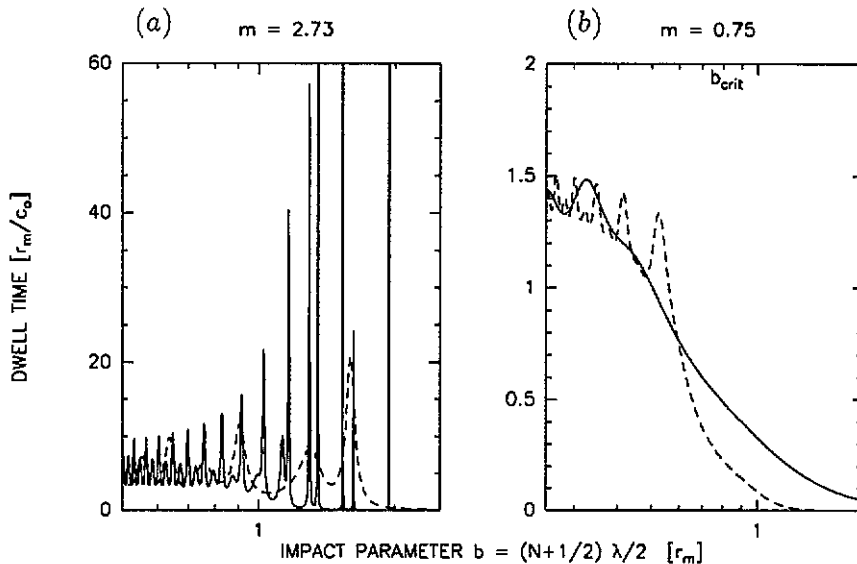


Figure 2. (a) Conditional dwell times per partial wave for a Mie sphere with index of refraction $m = 2.73$. The horizontal axis is labelled with the 'impact parameter' $b = (n + 1/2)\lambda/2\pi$ in geometrical optics, where n is the principal quantum number of the partial wave under consideration. Some specific values for n are plotted; bold: $n = 10$, dashed: $n = 2$. (b) As in (a) but for an index of refraction $m = 0.75$. The critical impact parameter is given by $b_{\text{crit}} = m$ beyond which one expects, according to ray optics, total reflection off the sphere.

Figure 2 shows the evaluation of this expression for an index of refraction $m = 2.73$ ('attractive') and $m = 0.75$ ('repulsive'). The horizontal axis is labelled with the parameter $(n + 1/2)\lambda/2\pi$, which can be recognized as the 'impact parameter' in the ray picture [26] and is inversely proportional to the frequency. The pronounced peaks correspond to *shape resonances*, i.e. the wave is trapped inside the Mie sphere, and a standing wave is built up. In some cases the dwell time exceeds the 'free time' r_m/c_0 by two orders of magnitude. Some very strong peaks arise for impact parameters $(n + 1/2)\lambda/2\pi > r_m$. This means that they are geometrically forbidden in the sense that rays with these impact parameters are not expected to be captured by the sphere.

These enormous dwell times will introduce a delay every time a scattering process takes place. In the case of multiple scattering, such a delay accumulates and becomes macroscopic (of the order of the mean free time), thereby giving rise to a decrease in the speed of light [8, 9].

We draw attention to a very convenient relation between absorption and dwell time, apparent from equation (66). Summing this result over all partial waves yields

$$W(B, E) = \frac{3}{8} \frac{m}{x} \lim_{m_i \rightarrow 0} \frac{Q_{\text{abs}}}{m_i} + \text{rest} \quad (67)$$

where Q_{abs} is the Quality factor for absorption, and is the absorption cross section normalized to πr_m^2 . The rest term is known explicitly, but turns out to be negligible near resonances. Accordingly, from equation (64) we obtain for the charging time,

$$\tau_B^c(E) \approx \frac{m}{E} \lim_{m_i \rightarrow 0} \frac{1-a}{2m_i} \quad (68)$$

We introduced the *albedo* a of the scatterer, $a \equiv 1 - Q_{\text{abs}}/Q_E$. Equation (68) can be reproduced heuristically [9]. Physically, it expresses the fact that the longer the light spends in the dielectric barrier, the more it will suffer from absorption. A similar, but *exact* formula can be derived for the case of Schrödinger potential scattering (appendix). The rest term in equation (67) is a manifestation of the so-called 'logarithmic derivative', causing different boundary conditions for the TE and TM modes in the sphere. The TM mode (with t -matrix a_n) is influenced by this term. The logarithmic derivative is absent for the TE mode.

5. A Jauch-type formula for scalar waves

In principle, our dynamic approach to the Maxwell equations in equation (39) is suited to formulating a Jauch formula for light. Although only valid for Schrödinger potential scattering, the proof of this formula given by Martin [6] shows its validity under very general conditions. We will not deal with polarization effects here. Instead, we derive a Jauch-type formula for the scalar wave equation (35), making use of the analogy of Schrödinger particles and scalar waves mentioned earlier;

$$-\frac{1}{2k^2} \frac{d}{dk} k \text{Re } t_{kk}(k^+) + \int d\hat{k}' \frac{|t_{kk'}(k)|^2}{(4\pi)^2} \frac{d\phi(k')}{dk} = \lim_{a \rightarrow \infty} [W_{kk}(B_a) - W_{kk}^0(B_a)]. \quad (69)$$

In this formula W_{kk} is the scalar counterpart of the definition equation (57), B_a is a sphere of radius a and $t_{kk'}(k^+)$ is the on-shell t -matrix associated with the scalar wave equation, and should, in turn, be considered as an analogue of equation (51). The left-hand side of equation (69) is proportional to the monochromatic phase-delay time in three dimensions, the first term being the contribution of the coherent channel, and the second term a summation over all scattering channels. Equation (69) can be derived as follows.

In the scalar wave equation (35) ψ plays the role of vector potential where the 'electric component' is $\partial_t \psi$ and the 'magnetic component' $\nabla \psi$. As mentioned in equation (37) we identify the 'energy' as E^2 and the 'potential' as $[1 - \epsilon(\mathbf{r})]E^2$. Having found the off-shell t -matrix $t_{kk'}(E^+, V_0)$ from the Schrödinger eigenvalue problem with potential $V_0 g(\mathbf{r})$, the t -matrix of the scalar wave equation is $t_{kk'}(E^2, V_0(E))$. Letting $E = k$ gives the on-shell t -matrix as above. The validity of the Jauch formula for Schrödinger particles guarantees that the partial derivatives at 'constant potential' give

$$-\frac{1}{2k^2} \left(\frac{\partial}{\partial k} \right)_{V_0} k \operatorname{Re} t_{kk}(k^+) + 2k \int d\hat{k}' \frac{|t_{kk'}(k^+)|^2}{(4\pi)^2} \left(\frac{\partial \phi(k')}{\partial k^2} \right)_{V_0} = \int d\mathbf{r} [|\varphi_k(\mathbf{r})|^2 - 1]$$

φ_k being a normalized continuum eigenfunction of the Schrödinger equation at eigenvalue $E = k^2$. On the other hand, it is shown in the appendix, in combination with equation (62), that the derivatives with respect to V_0 equal

$$-\frac{\partial}{\partial V_0} \operatorname{Re} t_{kk}(k^+) + 2k \int d\hat{k}' \frac{|t_{kk'}(k^+)|^2}{(4\pi)^2} \frac{\partial \phi(k')}{\partial V_0} = \int_B d\mathbf{r} [\epsilon(\mathbf{r}) - 1] |\varphi_k(\mathbf{r})|^2.$$

Since $V_0(E) = E^2$ we have $d/d(E^2) = (\partial/\partial E^2)_{V_0} + \partial/\partial V_0$ so that we obtain for the left-hand side of equation (69),

$$\int d\mathbf{r} [\epsilon(\mathbf{r})|\varphi_k(\mathbf{r})|^2 - 1] = \int d\mathbf{r} \left[\frac{1}{2} \epsilon(\mathbf{r})|\varphi_k(\mathbf{r})|^2 + \frac{1}{2E^2} |\nabla \varphi_k(\mathbf{r})|^2 - 1 \right].$$

This is recognized as the inner product (energy) for scalar waves [28] and equals, by definition, the right-hand side of equation (69). The last equality follows from $\nabla \cdot (\varphi^* \nabla \varphi) = |\nabla \varphi|^2 - E^2 \epsilon(\mathbf{r})|\varphi|^2$ for any $\varphi(\mathbf{r})$ obeying the time-independent scalar wave equation.

6. Conclusions

In this paper we have formulated the concept of a conditional dwell time. In one dimension a conditional dwell time probes the time that a wavepacket spends in the potential region *provided* it finally emerges in either the transmission or the reflection channel. For inversion symmetric potentials *and* in the monochromatic limit the conditional dwell time for both channels coincide with the 'unconditional' dwell time. All are given by the integral $W_{kk}(B)$ of the square of the continuum eigenfunction at energy $E = k^2$ over the potential region B . This matrix element was shown to be a (functional) derivative of the phase shift of the S -matrix with respect to potential, and is also intimately related to absorption arguments. It follows that $W_{k,-k}(B)$ provides additional information about the dynamics in the potential region.

Using a time-dependent theory for light propagation, we obtained expressions for the conditional dwell time for light emerging in an infinitesimal solid angle. We observed that a first-order dynamic approach to Maxwell's equations is consistent with the notion of an 'energy-dependent potential' in the classical (second-order) wave equations. This energy dependence makes the dynamics of light different from Schrödinger dynamics. In particular, derivatives with respect to potential enter into the phase-delay time of classical waves, making delay much more pronounced than in the quantum mechanical picture. We pointed out that the energy-dependent potential is consistent with the different conserved quantity associated with classical wave motion. A Jauch formula for classical waves is discussed in this context. We recently showed that the different conserved quantity in the classical wave equations gives rise to a substantial renormalization of the transport velocity in random media.

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Appendix. Dwell time in quantum mechanics

In this appendix we derive an expression for the dwell time in the case of Schrödinger potential scattering. Starting with the Schrödinger wave equation with a complex-valued potential,

$$i\nabla\psi(\mathbf{r}, t) = -\nabla^2\psi(\mathbf{r}, t) + V(\mathbf{r})\psi(\mathbf{r}, t)$$

we obtain the well known *equation of continuity*,

$$\nabla \frac{1}{2} |\psi(\mathbf{r}, t)|^2 + \nabla \cdot \mathbf{J} = \text{Im } V(\mathbf{r}) |\psi(\mathbf{r}, t)|^2 \quad (70)$$

with $\mathbf{J} = \text{Im } \psi^* \nabla \psi$. Finally we take the limit of the vanishing imaginary part. We define the linear functional,

$$\Phi[g] = \int_{-\infty}^{\infty} dt \int d\mathbf{r} g(\mathbf{r}) |\psi(\mathbf{r}, t)|^2 \quad (71)$$

where $g(\mathbf{r})$ is real-valued and has compact support. If $\text{Im } V(\mathbf{r}) = V_i g(\mathbf{r})$ we get

$$\Phi[g] = \lim_{V_i \rightarrow 0} \frac{1}{V_i} \int_{-\infty}^{\infty} dt \int dS \cdot \mathbf{J}(\mathbf{r}, t).$$

By Gauss' theorem, the surface integral can be performed on any sufficiently smooth closed surface surrounding the support of g . We shall work it out in three dimensions. The asymptotic (outgoing) solution of the Schrödinger equation is, in terms of the scattering amplitude $f_{\mathbf{k}}(\theta)$,

$$\psi(\mathbf{r}, t) = \sum_{\mathbf{k}} \psi_0(\mathbf{k}) \left[e^{i\mathbf{k} \cdot \mathbf{r}} - f_{\mathbf{k}}(\theta) \frac{e^{i\mathbf{k}r}}{4\pi r} \right] e^{-i\mathbf{k}^2 t} \quad (72)$$

with θ fixing the direction of \mathbf{r} . It follows, for $r \rightarrow \infty$,

$$\int_{-\infty}^{\infty} dt \hat{\mathbf{r}} \cdot \mathbf{J}(\mathbf{r}, t) = \pi \operatorname{Re} \sum_{\mathbf{k}\mathbf{k}'} \delta(\mathbf{k} - \mathbf{k}') \psi_0(\mathbf{k})^* \psi_0(\mathbf{k}') \left[e^{i(\mathbf{k}' - \mathbf{k}) \cdot \mathbf{r}} (\hat{\mathbf{r}} \cdot \hat{\mathbf{k}}') - e^{-i\mathbf{k} \cdot \mathbf{r}} \frac{e^{i\mathbf{k} \cdot \mathbf{r}}}{4\pi r} f_{\mathbf{k}'}(\theta) - e^{i\mathbf{k}' \cdot \mathbf{r}} \frac{e^{-i\mathbf{k}' \cdot \mathbf{r}}}{4\pi r} f_{\mathbf{k}}(\theta)^* (\hat{\mathbf{r}} \cdot \hat{\mathbf{k}}') + \frac{f_{\mathbf{k}}(\theta)^* f_{\mathbf{k}'}(\theta)}{(4\pi r)^2} + \dots \right].$$

Making use of the formal identity,

$$\lim_{r \rightarrow \infty} r e^{\pm i\mathbf{k} \cdot \mathbf{r}} \int_{-1}^1 dc F(c) e^{\mp i\mathbf{k} r c} = \frac{\pm i}{k} F(1) \tag{73}$$

where $c = \cos \theta$, we finally obtain

$$\Phi[g] = \pi \lim_{V_i \downarrow 0} \frac{1}{V_i} \operatorname{Re} \sum_{\mathbf{k}\mathbf{k}'} \psi_0(\mathbf{k})^* \psi_0(\mathbf{k}') \delta(\mathbf{k} - \mathbf{k}') \times \left[-\frac{i}{2k} (f_{\mathbf{k}'}(\hat{\mathbf{k}}) - f_{\mathbf{k}}^*(\hat{\mathbf{k}}')) + \int d\hat{\mathbf{r}} \frac{f_{\mathbf{k}}^*(\hat{\mathbf{r}}) f_{\mathbf{k}'}(\hat{\mathbf{r}})}{(4\pi)^2} \right].$$

This is further simplified by concentrating $\psi_0(\mathbf{k})$ in the element $d\mathbf{k} d\Omega$, while retaining its normalization. Upon introduction of the *functional derivative* [29]

$$\delta_V^\xi H[V] = \lim_{\Delta \downarrow 0} \frac{H[V(\mathbf{r}) + \Delta \xi(\mathbf{r})] - H[V(\mathbf{r})]}{\Delta} \tag{74}$$

where $\xi(\mathbf{r})$ can be complex-valued, we arrive at

$$\frac{d\Phi[g]}{d\Omega} = \frac{1}{2} \left(\frac{k}{2\pi} \right)^2 \delta_V^{ig} \left[\frac{1}{k} \operatorname{Im} f_{\mathbf{k}}(\hat{\mathbf{k}}) + \int d\hat{\mathbf{r}} \frac{d\sigma}{d\Omega} (\hat{\mathbf{k}} \rightarrow \hat{\mathbf{r}}) \right]. \tag{75}$$

Here $|f_{\mathbf{k}}(\hat{\mathbf{r}})|^2 / (4\pi)^2 \equiv d\sigma / d\Omega$, the differential cross section in the direction $\hat{\mathbf{r}}$. Equation (75) can be recognized as a derivative of the absorption cross section with respect to the imaginary part of the potential, similar to equation (67). Using the fact that $f_{\mathbf{k}}$ depends functionally on $V(\mathbf{r})$, whereas $f_{\mathbf{k}}^*$ depends on its complex conjugate, this can also be written as

$$\frac{d\Phi[g]}{d\Omega} = -\frac{1}{2} \left(\frac{k}{2\pi} \right)^2 \left[-\frac{1}{k} \delta_V^g \operatorname{Re} f_{\mathbf{k}}(\hat{\mathbf{k}}) + 2 \int d\hat{\mathbf{r}} \frac{d\sigma}{d\Omega} (\hat{\mathbf{k}} \rightarrow \hat{\mathbf{r}}) \delta_V^g \phi(\hat{\mathbf{r}}) \right]. \tag{76}$$

Here $\phi(\hat{\mathbf{r}})$ is the complex phase of the t -matrix in the direction $\hat{\mathbf{r}}$. Alternatively, equation (76) can be obtained from equation (75) by application of the Cauchy-Riemann equations. In one dimension there is no solid angle degeneracy and the result reads

$$\Phi[g] = -\frac{1}{2} \delta_V^{ig} [1 - |R(k)|^2 - |T(k)|^2] = -|R(k)|^2 \delta_V^g \phi_R - |T(k)|^2 \delta_V^g \phi_T. \tag{77}$$

Here $R(k)$ and $T(k)$ represent the complex reflection and transmission coefficients; ϕ_R and ϕ_T are their phase shifts.

We discuss two relevant choices for g . First, we can take $g(\mathbf{r})$ equivalent to the characteristic function $\chi_B(\mathbf{r})$ of the potential region. Then

$$\Phi[\chi_B] = \int_{-\infty}^{\infty} dt \int_B d\mathbf{r} |\psi(\mathbf{r}, t)|^2 = \tau_B \quad (78)$$

where τ_B is the dwell time analogous to equation (53). We conclude that the dwell time can be formulated in terms of a functional derivative with respect to the potential in the direction of its characteristic function. Another very interesting option is obtained by choosing g such that $V(\mathbf{r}) = V_0 g(\mathbf{r})$. The functional $\Phi[V]$ represents the potential energy integrated over time. Now the functional derivative δ_V^g reduces to an ordinary derivative d/dV_0 . Going to the plane-wave limit of $\Phi[V]$ in three dimensions, yields, in combination with equation (76),

$$\begin{aligned} \langle \varphi_k^+ | g | \varphi_k^+ \rangle &= \frac{d}{d(\text{Im } V_0)} \left[\text{Im } f_k(\hat{\mathbf{k}}) + k \int d\hat{r} \frac{d\sigma}{d\Omega}(\hat{\mathbf{k}} \rightarrow \hat{r}) \right] = -k \frac{d\sigma_{\text{abs}}}{d(\text{Im } V_0)} \\ &= \frac{d \text{Re } f_k(\hat{\mathbf{k}})}{dV_0} - 2k \int d\Omega \frac{d\sigma}{d\Omega} \frac{d\phi(\Omega)}{dV_0}. \end{aligned} \quad (79)$$

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