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# The influence functional: application to tunnelling

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**Abstract.** The influence functional is introduced as a kernel in an integral equation that gives the probability density at time $t$ and position $q$ in terms of the initial probability density. This functional is applied to tunnelling through a square barrier to determine the influence, at different times, of various regions of the incident packet on the transmitted peak.

## 1. Introduction

The primary object in the standard formulation of quantum mechanics is the probability *amplitude* $\psi(q)$. However, ordinary probabilities are usually easier to understand and handle. In fact the connection between the wave formalism and the particle concept is accomplished, via Born's postulate, by associating the square of $|\psi(q)|$ with the probability density of the particle's presence at $q$ [1]. The influence of the wavefunction at a spatial point $q_0$ at time $t_0$, on the wavefunction at a point $q$ at time $t$ is determined by a Green's function $G(q, t; q_0, t_0)$ (also called the 'propagator', 'transition amplitude', or 'influence function') in an integral equation involving amplitudes:

$$\psi(q,t) = \int G(q,t;q_0,t_0)\psi(q_0,t_0)\,\mathrm{d}q_0 \tag{1}$$

(the integrals go from $-\infty$ to $\infty$ throughout this work unless stated otherwise), where

$$G(q,t;q_0,t_0) = \langle q|\mathrm{e}^{-\mathrm{i}\hat{H}(t-t_0)/\hbar}|q_0\rangle \tag{2}$$

and $\hat{H}$ is the Hamiltonian. (A circumflex accent denotes quantum operators.) Here and in the following a structureless particle in one dimension is assumed for simplicity. Using (1) twice, the probability density, $P(q,t) = |\psi(q,t)|^2$, is *not* expressed as

$$P(q,t) = \int \mathcal{F}(q,t;q_0,t_0)P(q_0,t_0)\,\mathrm{d}q_0. \tag{3}$$

Instead, one finds 'non-diagonal' influences of different points, namely,

$$P(q,t) = \iint \mathrm{d}q'\,\mathrm{d}q''\,G(q,t;q',t_0)^*\psi(q';t_0)^*\psi(q'';t_0)G(q,t;q'',t_0). \tag{4}$$

There is, of course, nothing technically wrong with equation (4), but its interpretation in terms of particle probabilities becomes problematic because in the integrand there are only amplitudes. Is it possible to find an object $\mathcal{F}$ in (3) independent of the 'source function' $P(q_0,t_0)$ at least within a set of states? Such an $\mathcal{F}$ would allow the control of the future evolution of the system of interest by an appropriate localization of the initial state. (There

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are two known solutions for $\mathcal{F}$ in (3) within the framework of 'stochastic' [2] and 'casual' [3] interpretations of quantum mechanics. However, none of these solutions are independent of the particular initial state and, therefore, they are useless in this sense.)

The main objective of this paper is to describe an object, the *influence functional*, that answers positively our basic question asked above. It is a kernel, $\mathcal{F}$, in the integral equation (3) that gives a quantitative meaning to the influence of the probability for being at a given point at time zero, on the probability for the presence at a second point of space at a later time. The name 'functional' is due to the fact that different 'families' of initial states require different $\mathcal{F}$'s. Within the corresponding family, $\mathcal{F}$ is independent of $P(q_0, t_0)$, as it corresponds to a Green's function. (It is not, however, a true Green's function for reasons explained later.) As an application, we shall study tunnelling through a square barrier by determining the influences of various regions of the incident packet at different times on the transmitted peak.

Even though the concepts and techniques involved are valid generally, most of the discussion centres on packets that are initially Gaussian, which is the most widely assumed form for interpreting collision experiments or in numerical wave-packet computations. The wavepacket is always assumed to come from the left.

## 2. The influence functional: general theory

A direct comparison of the known expression (4) and the formula (3), which is our objective, may seem discouraging. Indeed, several quantities or formalisms were examined and discarded as candidates to account for the point-to-point influences we are looking for. However, one of the approaches, the Weyl–Wigner formalism, will lead naturally to the desired object.

The quantity

$$\langle q|e^{-i\hat{H}(t-t_0)/\hbar}|q_0\rangle\langle q_0|e^{i\hat{H}(t-t_0)/\hbar}|q\rangle \tag{5}$$

might have been considered relevant. After all, it gives the probability density at $q, t$ when the particle was originally at $q_0, t_0$. However, according to (4) this is clearly not sufficient to determine $P(q, t)$.

We may also investigate the correlation between being at $q_0$ at time $t_0$ and being at $q$ at time $t$ by means of the quantum correlation function

$$\langle\psi(t_0)|\delta(\hat{q}-q_0)e^{i\hat{H}(t-t_0)/\hbar}\delta(\hat{q}-q)e^{-i\hat{H}(t-t_0)/\hbar}|\psi(t_0)\rangle \tag{6}$$

$$= \langle\psi(t_0)|q_0\rangle\langle q_0|e^{i\hat{H}(t-t_0)/\hbar}|q\rangle\langle q|\psi(t)\rangle \tag{7}$$

where $\hat{q}$ is the position operator. However, since $\hat{q}$ and $\hat{H}$ do not commute, this is a complex quantity. The interpretation of real and imaginary parts is problematic [2, 4] and, in addition, it does not relate to an expression of the form (3) either.

The Bohm interpretation provides an equation of the form (3) [5–7]. In this interpretation the particles are well localized objects describing trajectories 'guided' by the wavefunction [3]. However, the kernel $\mathcal{F}_{\text{Bohm}} = \delta\{q_B[t; q_0, \psi(t_0)] - q\}$, where $q_B[t; q_0, \psi(t_0)]$ is, according to Bohm's prescriptions, the position at time $t$ of the particle that was initially at $q_0$, is completely dependent on the initial state $\psi(t_0)$ and lacks predictive power. This means that every initial state requires a recalculation of $q_B$. We shall return to this aspect in the final discussion.

Finally, in the Weyl–Wigner equivalent formulation of quantum mechanics there is a phase-space 'transition kernel' $T(q, p, t; q_0, p_0, t_0)$ that links the Wigner functions,

representing the state of the system, at $t_0$ and $t$. ($T$ is the quantum version of the classical kernel $K$, see (19) below. It is discussed in detail in [8].) This is in principle an interesting quantity because it is completely independent of the initial state. However, it is cumbersome from the point of view of the numerical computation, and in fact it carries too much information when compared with the coordinate space kernel $\mathcal{F}$. An integration over momenta is required. Instead of first calculating the phase space transition kernel $T$, an alternative route that avoids this step is now described.

Since much of the following theory is based on the Weyl–Wigner equivalent formulation of quantum mechanics, the basic elements of this formalism are briefly reviewed [9–12]. The Weyl transform $A_W$ of an operator $\hat{A}$ is a function of the phase-space variables $q, p$ defined by

$$A_W(q, p) \equiv \int \left\langle q - \frac{y}{2} \middle| \hat{A} \middle| q + \frac{y}{2} \right\rangle e^{ipy/\hbar}\, dy. \tag{8}$$

This representation of quantum operators allows us to express the quantum-mechanical trace of two operators, $\mathrm{tr}(\hat{A}\hat{B})$, as a phase-space integral of their Weyl transforms. In particular, the average of $\hat{A}$ is given by

$$\langle \hat{A} \rangle = \int\int W(q, p, t) A_W(q, p)\, dp\, dq$$

where the Wigner function $W$ is, up to a constant, the Weyl transform of the density operator $\hat{\varrho}$, i.e. $W = 1/(2\pi\hbar)\varrho_W$. In terms of the Wigner function, equation (4) can be written as

$$P(q,t) = \int\int\int dp_0\, dq_0\, dy\, W(p_0, q_0, t_0) G(q, t; q_0 - y/2, t_0)^* G(q, t; q_0 + y/2, t_0) e^{ip_0 y/\hbar}. \tag{9}$$

We now define the family of states $\{W_Q\}$ as the set of Wigner functions which share the same quotient

$$Q(q_0, p_0) = W_Q(q_0, p_0, t_0) / \int dp_0\, W_Q(q_0, p_0, t_0).$$

Using the fact that the *marginal* of the Wigner function is equal to the probability density, $Q$ can also be written as $Q = W_Q(t_0)/P(t_0)$. Since the Wigner function is normalized, $Q$ obeys

$$\int dp_0\, Q(q_0, p_0) = 1. \tag{10}$$

For Gaussian functions, $W$ is positive everywhere and $Q$ can be viewed as a conditional probability $Q(p_0|q_0)$; this is not a necessary condition for the validity of our results. Comparing (9) with (3), the influence functional is defined as

$$\mathcal{F}_Q(q, t; q_0, t_0) \equiv \int dy\, G(q, t; q_0 - y/2, t_0)^* G(q, t; q_0 + y/2, t_0) \int dp_0\, Q(q_0, p_0) e^{ip_0 y/\hbar}. \tag{11}$$

Taking the complex conjugate and changing the integration variable $y$ to $-y$, it is easily seen that $\mathcal{F}_Q(q, t; q_0, t_0)$ is a real quantity.

The influence functional $\mathcal{F}_Q$ fulfils some, but not all, of the properties of a Green's function. In particular, it does *not* obey a Chapmann–Kolmogorov type of equation, i.e. in general

$$\mathcal{F}_Q(q, t; q_0, t_0) \neq \int \mathcal{F}_Q(q, t; q', t') \mathcal{F}_Q(q', t'; q_0, t_0)\, dq'. \tag{12}$$

The reason being that the state at $t'$ will not in general belong to the initial family of states determined by $Q(q_0, p_0)$. The explicit dependence of $\mathcal{F}$ on $Q(q_0, p_0)$ has been included in (12) to illustrate this fact but will otherwise be omitted.

## 3. Factorized initial states

An important family of states is the set of Wigner functions having the structure

$$W(q_0, p_0, t_0) = P(q_0, t_0)\frac{2^{1/2}\delta}{\pi^{1/2}\hbar}\exp[-2\delta^2(p_0 - p_{00})^2/\hbar^2]. \tag{13}$$

These states have a Gaussian momentum distribution with mean $p_{00}$, variance $[\hbar/(2\delta)]^2$, and no correlation between $p_0$ and $q_0$. The minimum uncertainty Gaussian packets

$$\psi(q_0, t_0) = (2\pi\delta^2)^{-1/4}\exp[-(q_0 - q_{00})^2/4\delta^2]\exp[\mathrm{i}p_{00}(q_0 - q_{00})/\hbar] \tag{14}$$

with Wigner function

$$W(q_0, p_0, t_0) = \frac{1}{\pi\hbar}\exp[-(q_0 - q_{00})^2/2\delta^2]\exp[-2\delta^2(p_0 - p_{00})^2/\hbar^2] \tag{15}$$

having position and momentum widths (square root of the variances) $\delta$ and $\hbar/(2\delta)$ respectively, are particular cases of this family.

For this family the variables $p_0$ and $q_0$ are statistically independent so that $W(q_0, p_0, t_0) = Q(p_0)P(q_0, t_0)$, and $Q(p_0)$ becomes the initial momentum distribution. The integral over $p_0$ can be done explicitly in this case and the influence functional takes the form

$$\mathcal{F}(q, t; q_0, t_0) = \int \mathrm{d}y\, G(q, t; q_0 - y/2, t_0)^* G(q, t; q_0 + y/2, t_0)$$
$$\times \exp[(-y^2/8\delta^2) + (\mathrm{i}p_{00}y/\hbar)]. \tag{16}$$

Once this object is calculated, it has *predictive* capabilities. In particular, it establishes the optimal location of a minimum initial wavepacket with average momentum $p_{00}$ and momentum variance $[\hbar/(2\delta)]^2$ in order to obtain maximum probability of the presence in $q$ at time $t$. The probability density $P(q, t)$ is given by the overlap between this functional and the initial probability density $P(q_0, t_0)$.

In general the computation of (16) will be numerical, but in some special cases analytical results may be found.

### *3.1. Analytical examples*

For the free particle the propagator is known analytically:

$$G(q, t; q_0, t_0) = \langle q|\exp[-\mathrm{i}\hat{H}(t - t_0)/\hbar]|q_0\rangle = \left[\frac{2\pi\mathrm{i}\hbar(t - t_0)}{m}\right]^{-1/2}\exp\left[\frac{\mathrm{i}m(q - q_0)^2}{2\hbar(t - t_0)}\right] \tag{17}$$

which, for initial states of the form (13), gives the influence functional

$$\mathcal{F}(q, t; q_0, t_0) = \frac{2^{1/2}m\delta}{\pi^{1/2}\hbar(t - t_0)}\exp\left[-2\delta^2\left[\frac{m(q - q_0)}{t - t_0} - p_{00}\right]^2/\hbar^2\right]. \tag{18}$$

We shall also calculate the *classical* influence functional corresponding to the initial states given by (13) for a square barrier of potential energy $V_0$ between 0 and $d$ for later comparison with the quantum case. In this section we shall take advantage of the

similarities between the Weyl–Wigner formalism and classical statistical mechanics. The classical distribution function $f$ will play the role of the Wigner function. It obeys

$$f(q, p, t) = \iint \mathrm{d}q_0\, \mathrm{d}p_0\, K(q, p, t; q_0, p_0, t_0) f(q_0, p_0, t_0) \tag{19}$$

where $K(q, p, t; q_0, p_0, t_0) = \delta(q - q'')\delta(p - p'')$, and $q''$ and $p''$ are the position and momentum of the trajectory that started at $q_0$ and $p_0$ at time $t_0$, respectively. For $q_0 < 0$, $q \geqslant d$, $p_0 > p_b$ and for times larger than the critical time required to cross the barrier, $t - t_0 > \left(md/\sqrt{p_0^2 - p_b^2}\right) - q_0 m/p_0$,

$$q'' = d + \frac{p_0}{m}\left(t - t_0 - \frac{dm}{\sqrt{p_0^2 - p_b^2}} + \frac{q_0 m}{p_0}\right) \tag{20}$$

where $p_b = (2mV_0)^{1/2}$ is the barrier 'height' in momentum units. Integrating the classical phase-space distribution over $p$, assuming $q > d$, and assuming an initial state entirely localized on the left of the barrier, we obtain the probability density

$$\begin{aligned} P(q,t) &= \int f(q, p, t)\, \mathrm{d}p = \iiint \mathrm{d}q_0\, \mathrm{d}p_0\, \mathrm{d}p\, K(q, p, t; q_0, p_0, t_0) f(q_0, p_0, t_0) \\ &= \frac{2^{1/2}\delta}{\pi^{1/2}\hbar} \iiint \mathrm{d}q_0\, \mathrm{d}p_0\, \mathrm{d}p\, \delta(q - q'')\delta(p - p_0)\mathcal{H}(p_0 - p_b) P(q_0) \\ &\quad \times \exp[-2\delta^2(p_0 - p_{00})^2/\hbar^2] \\ &= \frac{2^{1/2}\delta}{\pi^{1/2}\hbar} \int \mathrm{d}q_0\, P(q_0) \int_{p_b}^{\infty} \mathrm{d}p_0\, \delta(q - q'') \exp[-2\delta^2(p_0 - p_{00})^2/\hbar^2] \end{aligned} \tag{21}$$

where $\mathcal{H}$ is the Heaviside step function. Under these conditions the influence functional is

$$\mathcal{F}_{\mathrm{class}}(q, t; q_0, t_0) = \frac{2^{1/2}\delta}{\pi^{1/2}\hbar} \int_{p_b}^{\infty} \mathrm{d}p_0\, \delta(q - q'') \exp[-2\delta^2(p_0 - p_{00})^2/\hbar^2]. \tag{22}$$

The integral can be performed with the aid of the delta function taking into account that $q''$ is a function of $p_0$:

$$\mathcal{F}_{\mathrm{class}}(q, t; q_0, t_0) = \frac{2^{1/2}\delta}{\pi^{1/2}\hbar} \frac{\exp[-2\delta^2(p_i - p_{00})^2/\hbar^2]}{[(t - t_0)/m] + p_b^2 d/(p_i^2 - p_b^2)^{3/2}}. \tag{23}$$

In this expression $p_i$ is the momentum satisfying the delta function $\delta(q - q'')$ (see (20)).

### *3.2. Numerical example*

Numerical calculations performed for a square barrier potential in the quantum case are now summarized. While some qualitative aspects of the following discussion are known or have been stated independently, we emphasize the quantitative character and the predictive capabilities of the present approach.

Influence functionals $\mathcal{F}(q, t; q_0, 0)$ for $p_{00} = 5$ (tunnelling) and $p_{00} = 9$ (above barrier) with $\delta = 2$, $p_b = 8$ and $t = 7$ have been calculated (atomic units are used throughout and $m = 1$) as a function of $q_0$, assuming the factorized form (13) for the initial state at time $t_0 = 0$. The position $q$ has been chosen as follows. Reference minimum Gaussian wavepackets (having $\delta = 2$) with $p_{00} = 5$ and $p_{00} = 9$ centred at $q_{00} = -20$ at $t = 0$ are evolved numerically with the square barrier potential [13]. At $t = 7$ the maximum value of the transmitted parts is respectively, at $q_5 = 15.6$ and $q_9 = 42.85$. These two values are

then used as the parameters to compute the quantum influence functionals with and without the square barrier, $\mathcal{F}_{sb}$ and $\mathcal{F}_{free}$ respectively. The classical influence functional, $\mathcal{F}_{class}$, is also obtained above the barrier (see figures 1(*a*) and 1(*b*)).

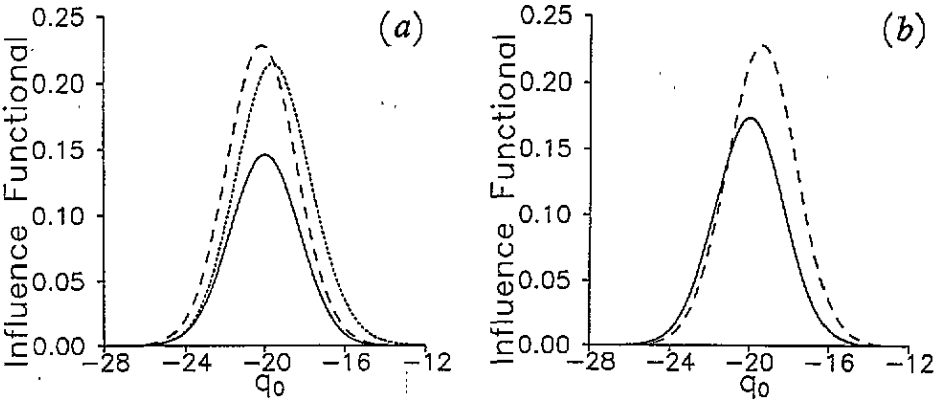


**Figure 1.** Influence functional $\mathcal{F}(q, t = 7; q_0, t_0 = 0)$ for initial factorized Gaussian states with $\delta = 2$ (atomic units in all figures). In (*a*) $q = 42.85$ and $p_{00} = 9$ and in (*b*) $q = 15.6$ and $p_{00} = 5$. Solid curves, quantum case corresponding to a square barrier between 0 and 1/2 with momentum height $p_b = 8$ (in (*b*) the value of this influence functional has been multiplied by a factor of 100); broken curves, free propagation (no barrier present); dashed curve, classical influence functional for the square barrier.

The important result is that $\mathcal{F}_{sb}$ is symmetrical with respect to $q_0 = -20$ in both cases: the front of the reference packet contributes as much as the rear to the transmitted peak, and the main contribution to the transmitted peak arises from the initial peak. This balance would be broken by displacing $q_{00}$ (which can be regarded as a control parameter): for initial positions closer to the barrier, $q_{00} > -20$, the rear would contribute more to the density at the chosen values of $q$ and $t = 7$; for more distant initial positions ($q_{00} < -20$) the front would contribute more. However, when $q_{00}$ deviates from $-20$, $P(q, t)$ decreases. Fixing $q_{00}$ at $-20$ and taking the spatial variance of $P(q_0, 0)$ as a control parameter, the calculated $\mathcal{F}_{sb}$ implies that the density $P(q, t)$ will decrease for an increasing spatial variance because of the smaller overlap between the functional and $P(q_0, 0)$.

Compare the ordering of the positions of the maxima (denoted as $\tilde{q}$) of the influence functionals for free propagation, $\tilde{q}_{free}$, and for the quantum square barrier case, $\tilde{q}_{sb}$: above the barrier ($p_{00} = 9$), $\tilde{q}_{free} < \tilde{q}_{sb}$; below the barrier ($p_{00} = 5$), $\tilde{q}_{sb} < \tilde{q}_{free}$. These maxima move to the right when $t < 7$ and to the left when $t > 7$. The classical case is a useful reference for transmission dominated by momenta above the barrier. In this case the quantum and classical propagations are quite similar [14, 15]. The crossing of a square barrier by a *classical* ensemble with non-zero momentum width implies two opposite effects in the velocities: At the barrier, the 'to be transmitted particles' are slowed down with respect to their free motion. However, the transmitted packet emerging from the barrier is on average faster than the incident packet because the filtering of momenta performed by the barrier and as a consequence, if $q$ is close enough to the barrier, the classically transmitted peak will always be delayed with respect to the peak of a packet propagated without a barrier. (Without a barrier, classical and quantum packets with identical initial conditions in phase space remain identical at all times.) This is reflected in the advanced position of the maximum of the classical influence functional $\tilde{q}_{class}$ with respect to $\tilde{q}_{free}$ for $p_{00} = 9$, $\tilde{q}_{free} < \tilde{q}_{class}$, in figure 1(*a*). The same is true quantally, namely $\tilde{q}_{free} < \tilde{q}_{sb}$. The order

$\tilde{q}_{sb} < \tilde{q}_{class}$ is due to a more severe filtering of the barrier in the quantum case.

The collision we examine below the barrier is an example of the *Hartman effect* [16]. Hartman discussed several regimes depending on the barrier width and the incident energy for packets with an initially sharp energy distribution. (He restricted the momentum width of these packets and made it linearly dependent on the average momentum $p_{00}$.) The interesting regime corresponds in the general case (for arbitrary Gaussian packets) to a plateau of the average time of arrival at point $d$, $\langle t \rangle_d^{out}$, as a function of packet width $\delta$, and barrier width $d$, (see figure 2) [17, 18]. The domain of the plateau region has been quantitatively delimitated in our previous work [17].

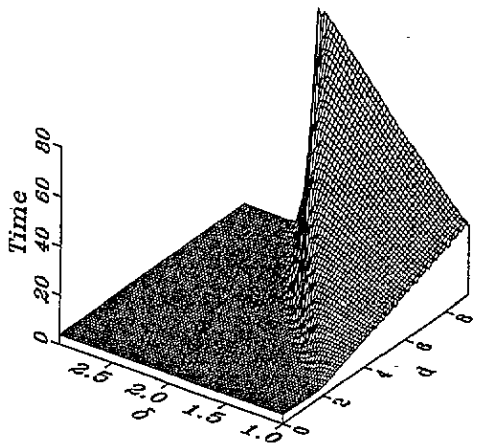


**Figure 2.** Average arrival time at the right barrier edge $d$ against $d$ and $\delta$ for $p_b = 8$, $q_{00} = -20$, $p_{00} = 5$.

An important feature of the propagation is that the probability density of the front of the free packet is always larger in our numerical calculations than the probability density of the transmitted packet, even if the transmitted peak is advanced with respect to the free peak. Thus, a mere comparison of peaks is clearly not telling the full story. A free packet would provide more particles arriving at an ideal detector at short times than a packet going through a barrier. Similar considerations apply for the influence functional: even though the relation $\tilde{q}_{sb} < \tilde{q}_{free}$ holds, the influence of any point $q_0$ in figure 1(*b*) in the free case is significantly larger than the influence for the barrier case.

In summary, the quantum influence functional valid for a family of minimum packets with fixed momentum distribution that collide with a square barrier has been calculated and compared with classical results and free propagation, for energies above and below the barrier. As a function of the initial coordinate $q_0$ this functional is symmetrical with respect to the value of the maximum (at least to numerical accuracy) and it allows the prediction of $P(q, t)$ by modifying the parameters of the initial position distribution $P(q_0, t_0)$. It has been shown that the peak of the transmitted packet is influenced the most by the peak of the initial packet.

## 4. Influence functional for general (correlated) Gaussians

We shall obtain the influence functional with the general Gaussian

$$W(q_0, p_0, t_0) = C \exp[-\tfrac{1}{2}A_{11}q_0^2 - \tfrac{1}{2}A_{22}p_0^2 - A_{12}q_0p_0 - B_1q_0 - B_2p_0] \quad (24)$$

as the initial state. $C$ is a normalization constant

$$C = (2\pi)^{-1}(\mathrm{Det}\,\mathbf{A})^{1/2}\mathrm{e}^{-BA^{-1}B/2} \tag{25}$$

$\mathbf{A}$ is a $2\times 2$ symmetric real matrix with positive diagonal elements, and $B$ is a vector with two components. Not every Gaussian function given by (24) is a valid quantum state. The uncertainty principle has to be satisfied, which implies [19]

$$4 \geqslant A_{11}A_{22} - A_{12}^2 > 0. \tag{26}$$

Integrating over $p_0$, the corresponding marginal distribution takes the form

$$P(q_0, t_0) = C\left(\frac{2\pi}{A_{22}}\right)^{1/2}\exp\left(\frac{B_2^2}{2A_{22}}\right)\exp\left[-q_0^2\left(\frac{A_{11}}{2} - \frac{A_{12}^2}{2A_{22}}\right) - q_0\left(B_1 - \frac{A_{12}B_2}{A_{22}}\right)\right]. \tag{27}$$

$Q(p_0|q_0)$ is obtained by dividing (24) by (27). Note that the resulting expression for $Q(p_0|q_0)$ is independent of $A_{11}$ and $B_1$ and, therefore, $P(q_0, t_0)$ may always be chosen with arbitrary mean and variance for a given $Q$ (provided that the resulting Wigner function is a valid quantum state). Performing the integration over $p_0$ in (11), the influence functional takes the form

$$\mathcal{F}(q, p; q_0, p_0) = \int \mathrm{d}y\, G(q, t; q_0 - y/2, t_0)^* G(q, t; q_0 + y/2, t_0) \times \exp\left[-\frac{y^2}{2A_{22}\hbar^2} - \frac{\mathrm{i}(A_{12}q_0 + B_2)y}{A_{22}\hbar}\right] \tag{28}$$

which is independent of the Gaussian parameters $A_{11}$ and $B_1$. If we restrict ourselves to pure states, the conditional probability $Q(p_0|q_0)$ starts depending on $q_0$ as soon as the minimum packet (15) evolves in time. Provided the wavepacket has minimum uncertainty product at $t = 0$, then

$$W(q_0, p_0, t_0) = \frac{1}{\pi\hbar}\exp\left[-\frac{(q_0 - p_0t_0/m - q_{00})^2}{2\delta^2}\right]\exp\left[-\frac{2\delta^2}{\hbar^2}(p_0 - p_{00})^2\right]. \tag{29}$$

Taking this correlated Gaussian state as the 'initial state', then the influence functional is a particular case of (28).

Comparing (29) with (24) we may identify the matrix $\mathbf{A}$ and vector $B$ components as

$$\begin{aligned} &A_{11} = \delta^{-2} \qquad A_{22} = (t_0/m\delta)^2 + (2\delta/\hbar)^2 \qquad A_{12} = -t_0/(m\delta^2) \\ &B_1 = -q_{00}/\delta^2 \qquad B_2 = t_0q_{00}/(m\delta^2) - p_{00}(2\delta/\hbar)^2. \end{aligned} \tag{30}$$

If $B_2$, $t_0$ and $\delta$ are kept fixed, the density functional built for this initial state is also valid for any state at $t_0$ that *was* centred in phase space at time zero (when the packets are minimum) along the line

$$p_{00} = -\frac{\hbar^2 B_2}{4\delta^2} + \frac{t_0\hbar^2}{4m\delta^4}q_{00}. \tag{31}$$

The information we obtain here is, therefore, complementary to the information obtained from the factorized case, where $p_{00}$ was kept fixed within a family of initial states.

In figure 3 the asymmetric influence functional $\mathcal{F}(q, t; q_0, t_0)$ for $Q(p_0|q_0)$ taken from an evolved, correlated Gaussian is shown as a function of $q_0$. $q$ and $t$ are chosen at the transmitted peak corresponding to a reference packet, $|G(t)\rangle$, that was a minimum Gaussian at $t = 0$. The function $Q(p_0|q_0)$ at $t_0 > 0$ is obtained from $|G(t_0)\rangle$, when position-momentum correlations are not zero. The shape of the 'initial' state at $t_0$, $|\langle q_0|G(t_0)\rangle|^2$, is also shown. (See details of the numerical data in the figure caption.) Now the front of the

*evolved* packet contributes more than the rear. This result is in *qualitative* agreement with Bohm's theory [20], or with a heuristic classical-like argument: quantum packets evolving under free motion are, when expressed in phase space as Wigner functions, identical to the distribution functions of the corresponding classical ensembles at all times. In classical propagation, as time passes the fast particles advance more than the slow particles and the front of the packet becomes predominantly populated by them. The front part can, therefore, (here the argument becomes non-rigorous and heuristic) be expected to contribute more to the transmitted peak.

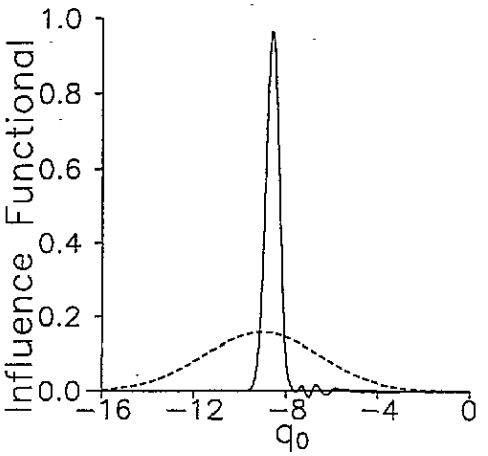


**Figure 3.** Influence functional $\mathcal{F}(q = 0.5, t = 7.954; q_0, t_0 = 6.19)$ (solid curve) for the function $Q(p_0|q_0)$ corresponding to a Gaussian packet at $t_0 = 6.19$ that was a minimum at $t = 0$. The probability density of this packet at $t_0$ is also shown (broken curve). At $t = 0$ this packet is centred at $p_{00} = 5$ and $q_{00} = -40$ in phase space. A square barrier potential is present between 0 and $d = 1/2$, with $p_b = 8$.

In this calculation the influence functional is much sharper than the Gaussian packet $\langle q_0|G(t_0)\rangle$, and selects a well localized portion, relatively close to the peak, of this initial state. In contrast, the widths of the influence functionals and the widths of the initial Gaussians that were used to determine $q$, $t$, and $Q(p_0|q_0)$ in the factorized Gaussian case of the previous section are very similar, so that the influence was more broadly distributed in that case.

Note that the influence functional may be negative at some points in figure 3, but that the overlap of this functional with any of the states in its domain of applicability always gives, because of its definition, a positive probability density (see equations (3) and (11)).

## 5. Discussion

We have given a quantitative meaning to the influence of the probability of the presence of a particle at a point on its future probability of being at a (generally) different point by means of the influence functional. It is, in general, a tool to control collision processes where the timing of the scattered part is of interest, for example to interact optimally with another prepared particle, or with a localized radiation source. The present study has paid attention to the probability density $P(q, t)$; an analogous treatment is possible for other quantities. For example, generalized influence functionals could be constructed by means of the Weyl–Wigner formulism to optimize the probability for the presence of the particle in a *region*

$q_i < q < q_f$, or to optimize the overlap with a particular state $\phi$. The initial state considered can be arbitrary but its associated influence functional has a domain of applicability, i.e. it is valid within a set of initial states. It has been shown that the functional takes simple forms for Gaussian states.

The influence functional has been applied to determine the effect of different parts of the initial wavepacket on the peak of the packet transmitted (via tunnelling) through a potential barrier [21–28]: paradoxically, some authors recognize that 'we cannot easily assign a portion of the incident wave to each portion of the transmitted wave', or that 'there is no meaning to the question of which part of the wavepacket gives rise to a given detection event', but simultaneously express the belief that (when the incident wave has evolved and developed position and momentum correlations) 'the peak that emerges consists primarily of what was originally in front', as a possible explanation of the Hartman effect [22, 25]. Many of these qualitative statements are too vague and unsatisfying as recognized by Landauer [22] for example. Our theory provides a definite framework (within sets of initial functions) in which these statements can be quantitatively tested. In particular it has been shown that (i) the influence functional for the transmitted peak position in a collision involving tunnelling does not favour rear or front tails of an initial minimum uncertainty packet and that (ii) when the minimum packet starts to evolve and develops position-momentum correlations, the front tail becomes more important.

Does this analysis clarify the paradoxical aspects of the Hartman effect? It certainly makes the type of assertion that one can make about influences of different packet regions more precise, but in this particular context we would rather stress the limitations of the concept of 'influence'. Different mathematical solutions exist for the kernel $\mathcal{F}$ in equation (3), all of them leading to the same probability density. Do any of them reflect a deeper physical reality? Our present understanding of quantum mechanics does not provide an answer. Some theories (stochastic or Bohmian mechanics) try to *explain* the influence in terms of trajectories; we do not attempt to do so with the influence functional. Instead, it is constructed as an operational tool, and this is its advantage over the other formal solutions.

The first result (i) is seemingly in contradiction with Bohm's theory, which assigns the transmitted peak to a point of the front tail of the (minimum) *initial* packet. Let us emphasize that both pictures are *formally* correct, and we do not question the validity of Bohm's results in this sense. We cannot honestly infer from the present work that Bohm's *physical picture* (in terms of causal trajectories) is wrong either. However, we claim that independently of the possible existence of a physical trajectory substratum of standard quantum mechanics, the influence functional is to be preferred for practical reasons. The important difference is that, if the influence functional is known, there is no need to re-calculate the wavepacket propagation to predict exactly the value of the probability density $P(q, t)$ when the initial state is changed. This means that the influence functional $\mathcal{F}_Q$ is—within its domain $\{W_Q\}$—independent of the initial state and, therefore, has a predictive power that Bohm's picture lacks. In Bohm's theory there is, strictly speaking, no influence of a point, but rather an influence of a point *conditioned to a particular quantum state*. In our approach, the influence of the state has been minimized and the conditioning is less severe, namely, each influence functional is valid for a family of initial states. Fortunately, there are families of states of practical interest. Thus, all non-correlated packets with common momentum distribution belong to the same family.

The reasons why some caution is required in not over-interpreting the results of the present analysis are clear: the influence functional is not a transition probability for particles since it does not obey a Chapman–Kolmogorov equation and it can be, in principle, negative. We can assert, for example, that when using minimum packets as initial states, a given

probability density at $q_0, t_0$ is 'causing' (in a statistical sense [29]) the presence of particles at $q, t$ with a weight determined by the influence functional. However, this particular 'causal' relation does not imply trajectories, nor does it give the right to say that the same particles that were at $q_0$ will later be at $q$ with probability $\mathcal{F}_Q(q, t; q_0, t_0)$, no matter how tempting this interpretation may be. In this regard, it is worthwhile recalling the status of the Wigner function. This is a perfectly respectable quantity useful in a variety of applications, and when properly averaged with Weyl transforms of operators associated with physical observables provides correct expectation values, even though there is no physical interpretation, in general, for its value (which can also be negative) at a phase-space point. In the same vein, the 'influences' that we are considering in this paper are to be understood operationally as useful intermediate objects under an integral sign in equation (3). If one is interested in maximizing, minimizing, or fixing the value of $P(q, t)$ the influence functional $\mathcal{F}_Q$ indicates how much weight each of the initial points will contribute to this integral when the initial state belongs to the set $\{W_Q\}$.

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## References

[1] The orthodox (Copenhagen) formulation of this postulate associates $|\psi(q)|^2$ with the probability density of 'finding' the particle (in an ideal measurement) at $q$, and denies physical reality to the presence of the particle before a position measurement is made. This view, however, is not necessarily accepted by all physicists, see e.g. Home D and Whitaker M A B 1992 *Phys. Rep.* **210** 223. The formalism and conclusions to be drawn from the present work are not affected by this controversial aspect. A 'Copenhagenist' should understand an expression such as 'the influence of the probability of the presence of the particle...' as 'the influence of the probability of finding the particle...' whenever it appears in the text.

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[13] These wavepackets at time $t = 0$ have a negligible component of negative momenta and can be considered as essentially asymptotic states; see Muga J G, Brouard S and Snider R F 1992 *Phys. Rev.* A **47** 6075. The scattering formalism then allows us to reduce the computation of $\psi(t)$ to the quadrature $\psi(x) = \int_0^\infty \mathrm{d}p\, \mathrm{e}^{-\mathrm{i}E_p t/\hbar}\langle x|p^+\rangle\langle p|\phi\rangle$, where $\langle p|\phi\rangle$ is the momentum representation of the initial state.

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[20] In Bohm's theory the initial point (at time $t_0$) linked by a causal trajectory to the position of the transmitted peak is in the very front tail of the initial packet, i.e. it is displaced to the right with respect to the region selected by our influence functional.

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[29] What does 'causal' mean? It was repeatedly argued by the founders of quantum mechanics that this theory is not causal. Frequently, it is understood that 'causal' has to do with 'trajectories'. In this respect the standard interpretation of the theory is not causal, but Bohm's theory is a 'causal interpretation' involving trajectories. In more general terms, causal means 'connected by a relationship of cause and effect', (no trajectory is required) and the 'cause' of an effect is the thing that makes it happen. In this sense quantum theory is at least statistically causal, since the initial states determine the future values of observables probabilistically. (Yet, in a relativistic context 'causal' is associated with Einstein's causality.)