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Collisional Transitory Enhancement of the High Momentum Components of a Quantum Wave Packet

S. Brouard and J. G. Muga

Departamento de Física Fundamentally Experimental, Universidad de La Laguna, La Laguna, Tenerife, Spain

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A classically forbidden, transitory enhancement of the high positive momentum components of a quantum wave packet during its collision with a potential barrier is described. A quantity is defined to measure its importance; the universality of the effect is justified, and its main features are studied with the aid of an analytically solvable model. Its relation to other "anomalously high velocities" is also examined. [S0031-9007(98)07182-8]

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Quantum mechanics may be cast as a *wave* theory. The "classically forbidden effects," such as tunneling, interferences, or the discretization of allowed values of certain observables, which are frequently regarded as distinctive signatures of quantum mechanics, are in fact common elements of all wave phenomena, classical or quantum. The counterintuitive and nonclassical aspects of these effects are revealed when the comparison is made instead with the behavior of classical *particles*. This comparison is legitimate since, behind the wave framework, quantum theory deals with particles, according to Born's interpretational postulate of the wave function.

The aim of this Letter is to disclose and analyze one of such classically forbidden effects that has remained essentially unnoticed in spite of being a universal feature of all scattering events: It is the transient, classically forbidden, collisional enhancement of high momentum components of a wave packet. Such a long disregard (we do not know of any work devoted to its description or study) may seem surprising after almost a century of scrutiny of quantum effects. The reason is surely related to an old and persistent prejudice that emphasizes the role of scattering theory as a link between asymptotic regimes, well before and well after the interaction is effective, and views the processes during the collision itself as irrelevant, because "they cannot be observed." This is not true anymore. Modern pulsed lasers allow one to probe the wave-packet dynamics, and techniques such as the "spectroscopy of the transition state" are but observations of reactive systems in the midst of a collision. Irrespective of being observed or not, the collisional regime has to be understood to ascertain, and eventually control, the mechanisms leading to the final products.

The simplest version of the effect implicates a one particle wave packet colliding with a potential barrier in one dimension, but the enhancement is also present in more general collisions. Let us consider an ensemble of classical particles of mass m in one dimension, described by the phase space distribution function $f(x, p; t)$, that collide with a potential $V(x)$, bounded from below, which we assume for simplicity to be nonzero only between $x = 0$ and $x = a$ (atomic units are used for all numerical values and figures, whereas the analytical expressions are valid for any system of units, so that $\hbar$ will be kept explicitly in quantum equations). Initially ($t = 0$), the ensemble is prepared to the left of the potential and with a negligible probability of negative momenta. The momentum of one particle along its trajectory, $p(t)$, can only be smaller than or equal to the initial one, $p(0)$, plus the momentum p_v due to the possible conversion from potential to kinetic energy,

$$p_v = \begin{cases} (-2mV_{\min})^{1/2} & \text{if } V_{\min} < 0\,, \\ 0 & \text{otherwise,} \end{cases} \quad (1)$$

where $V_{\min}$ is the minimum value of $V(x)$. Thus, as a consequence of energy conservation, the accumulated probability of momenta above $p + p_v$ at time $t > 0$ cannot exceed the initial accumulated probability above p,

$$G^{\rm cl}(p,t) \equiv \int_p^\infty \{P(p' + p_v, t) - P(p',0)\}\, dp' \le 0\,, \tag{2}$$

where $P(p',t) \equiv \int_{-\infty}^{\infty} f(x,p';t)\,dx$. Quantally, however, a similar bound cannot in general be established. We will study below examples where the quantity

$$G^{\rm q}(p,t) \equiv \int_p^\infty \{|\psi(p' + p_v, t)|^2 - |\psi(p',0)|^2\}\, dp'$$

takes on positive values. Figure 1 shows $|\psi(p,t)|^2$ and $|\psi(p,0)|^2$ as functions of p, for a time $t = 2.5$ during the collision of a Gaussian wave packet,

$$\psi(p,0) = \left(\frac{2\delta^2}{\pi\hbar^2}\right)^{1/4} e^{-i(p-p_c)x_c/\hbar} e^{-(p-p_c)^2\delta^2/\hbar^2}, \tag{3}$$

with an infinite wall (see the figure caption for details). In this case $p_v = 0$. The enhancement can be observed for momenta larger than $p \simeq 20.6$ (for $\delta = 2$), or larger than $p \simeq 21.3$ (for $\delta = 1$), where the momentum distributions of the wave packet at time t are above the initial distributions. Consequently, the accumulated increments of norm, $G^{\rm q}(p,t)$, for $t = 2.5$, have a maximum at $p \simeq 20.6$ (for $\delta = 2$), and at $p \simeq 21.3$ (for $\delta = 1$), as can be seen in Fig. 2, where a contour plot of the positive part of $G^{\rm q}(p,t)$ is represented as a function of p and t for the same collisions examined in Fig. 1. Dimensional analysis shows that once x_c/δ is fixed, the maximum value of $G^{\rm q}$ can depend only on $p_c\delta/\hbar$. In Table I the maximum value of $G^{\rm q}$ is given for several values of $p_c\delta/\hbar$ corresponding to $x_c/\delta = -25$, which is the value used in Figs. 1 and 2 for $\delta = 2$.

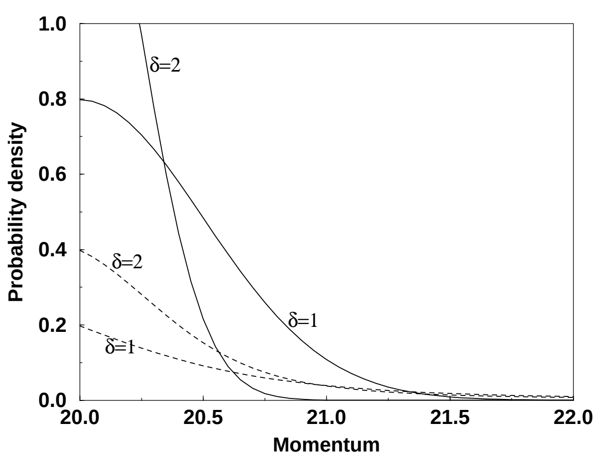

FIG. 1. $|\psi(p,t)|^2$ (dashed line) at time $t = 2.5$, and $|\psi(p,0)|^2$ (solid line), vs momentum, as given by Eqs. (8) and (3), respectively, with $p_c = 20$, $x_c = -50$, and several values of δ, indicated in the figure.

An important element of the effect apparent in Fig. 2 is its transitory nature. It disappears before and after the collision. Initially, $G^{\rm q}(p, t = 0) = 0$, whereas as $t \to \infty$,

$$|\psi(p, t \to \infty)|^2 \le |\psi(p, t = 0)|^2 \qquad (p > 0)\,, \tag{4}$$

since the S matrix commutes with the kinetic energy operator, and the probability of finding momentum p or $-p$ $(p > 0)$ is conserved from the initial to the final asymptotic states,

$$|\psi(p, t \to \infty)|^2 + |\psi(-p, t \to \infty)|^2 = |\psi(p, t = 0)|^2 \qquad (p > 0)\,. \tag{5}$$

The inequality of Eq. (4) implies that $G^{\rm q}(p,t)$ tends to a nonpositive value as $t \to \infty$.

We have also noticed this effect in collisions with different potentials, with and without discontinuities, local or nonlocal, with finite or infinite support, that can be studied analytically (the delta function and separable potentials), or numerically (Gaussian potentials and "square" barriers). Significant values of $G^{\rm q}$ can be achieved ($G^{\rm q} > 0.05$ in Fig. 2). In fact we shall argue that the effect is a universal feature of all collisions. Its origin can be traced back to the building blocks of the time-dependent wave packet, the stationary wave functions $|p'^{+}\rangle$. These are non-normalizable solutions of the Schrödinger equation corresponding to energy $E_{p'} = p'^2/2m$, an incoming plane wave $\langle x|p'\rangle = h^{-1/2}\exp\times(ip'x/\hbar)$, and outgoing boundary conditions for the scattered wave. In coordinate representation, if the potential $V(x)$ is restricted to the spatial interval $[0,a]$, the state $|p'^{+}\rangle$ can be written as

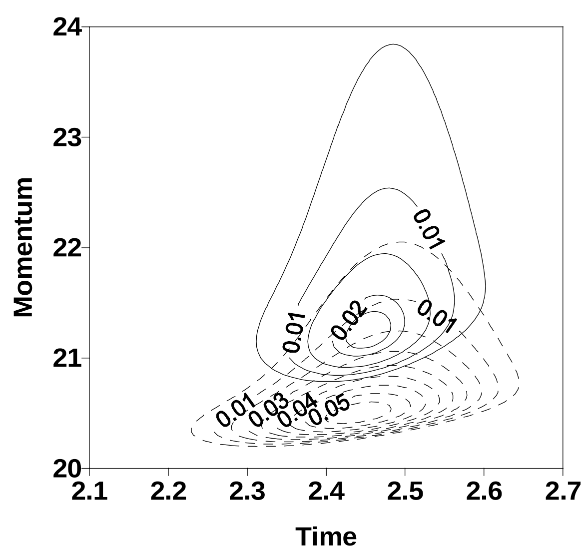

FIG. 2. Contour plot of the positive part of $G^{\rm q}(p,t)$ vs time and momentum, for an initial Gaussian wave packet (3) characterized by $p_c = 20$, $x_c = -50$, and $\delta = 1$ (solid lines) or $\delta = 2$ (dashed lines).

TABLE I. Maximum of G^{q} as a function of the dimensionless product $p_c\delta/\hbar$ for $x_c/\delta = -25$.

$p_c\delta/\hbar$	5.0	10.0	15.0	20.0	25.0	30.0	35.0	40.0	45.0
max(G^{q})	0.009	0.022	0.032	0.040	0.045	0.049	0.052	0.055	0.056

$$\langle x|p'^{+}\rangle = \begin{cases} h^{-1/2}[e^{ip'x/\hbar} + R(p')e^{-ip'x/\hbar}], & \text{if } x < 0\,, \\ h^{-1/2}T(p')e^{ip'x/\hbar}, & \text{if } x > a\,, \\ \chi(p',x), & \text{if } 0 < x < a\,, \end{cases} \tag{6}$$

where $R(p')$ and $T(p')$ are, respectively, the reflection and transmission amplitudes, and $\chi(p',x)$ is the solution in the interaction region. The Fourier transform of $\langle x|p'^{+}\rangle$ is given by the following distribution:

$$\langle p|p'^{+}\rangle = \frac{1}{2}[1 + T(p')e^{i(p-p')a/\hbar}]\delta(p - p') + \frac{i}{2\pi}[1 - T(p')e^{i(p-p')a/\hbar}]\mathcal{P}\left(\frac{1}{p - p'}\right) + \frac{1}{2}R(p')\left[\delta(p + p') + \frac{i}{\pi}\mathcal{P}\left(\frac{1}{p + p'}\right)\right] + \tilde{\chi}(p',p)\,, \tag{7}$$

where $\mathcal{P}$ denotes the Cauchy principal value. The principal value term $\mathcal{P}[1/(p' - p)]$ has a long tail that extends to infinity from the critical point $p = p'$, and the term $\tilde{\chi}(p',p) \equiv h^{-1/2}\int_0^a \chi(p',x)e^{ipx/\hbar}\,dx$ behaves, for nonvanishing $\chi(p',x)$, as p^{-1} when $p \to \infty$. These tails, which do not in general cancel each other, lead to nonzero amplitudes for classically forbidden values of p. Contrast this with a stationary flux of classical particles with incident momentum p'. In the classical context there cannot be momenta above $p' + p_v$. Even though the equation (7) justifies the universality of the effect [1], it represents a stationary state, so it cannot describe its time dependence and transient nature.

To illustrate and analyze the effect in the time-dependent case, we shall turn back to the simple example of Figs. 1 and 2. The temporal evolution of the wave function in momentum representation can be written in terms of w functions [2] as

$$\psi(p,t) = \frac{1}{2}\left(\frac{2\delta^2}{\pi\hbar^2}\right)^{1/4}\exp\left\{\frac{ip_cx_c}{\hbar} - \frac{p_c^2\delta^2}{\hbar^2} + \frac{b^2}{4a}\right\} \times [w(z_+) - w(z_-)]\,, \tag{8}$$

where $w(z) \equiv e^{-z^2}\,\mathrm{erfc}(-iz)$, and

$$z_\pm \equiv [p \pm b/2a]\sqrt{-a}\,, \tag{9}$$

$$b \equiv 2p_c\delta^2/\hbar^2 - ix_c/\hbar\,, \tag{10}$$

$$a \equiv -it/2m\hbar - \delta^2/\hbar^2. \tag{11}$$

Each collision can be defined by the parameters p_c, x_c, and δ, and studied as p and t vary, by analyzing a contour plot of $G^{\mathrm{q}}(p,t)$, as in Fig. 2. Even though G^{q} is the quantitative measure of the effect, it involves in general multiple integrals, also for analytical models, that make the prediction of its value or simple approximated analysis cumbersome. The characterization of the enhancement can be simplified by considering the ratio $\eta \equiv |\psi(p,t)|^2/|\psi(p,0)|^2$, between the momentum distributions with and without potential barrier. Unless p_c is very low, we are interested in momenta p where $w(z_-)$ represents only a small correction to $w(z_+)$, and can be neglected. Using Eqs. (3) and (8) one obtains

$$\eta(z_+) = \frac{1}{4}\left|\frac{w(z_+)}{\exp(-z_+^2)}\right|^2 = \frac{1}{4}|\mathrm{erfc}(z_+)|^2. \tag{12}$$

In other words, the ratio η has been reduced to the square modulus of the complementary error function computed at z_+, a dimensionless quantity that depends on the variables p, t, and the parameters p_c, x_c, and δ; see (9). This enables us to study the effect by drawing the contour plot of the function $\eta(z)$ in the complex z plane (in Fig. 3 using $\log_{10}[\eta(z)]$), and following the "trajectory" of z_+ as one of the variables or parameters of interest varies. Prominent features of the $\log_{10}[\eta(z)]$ function are two hills at right and left, a plateau around the negative imaginary z axis, and a valley for positive imaginary z. For a given initial wave packet, z_+ can be represented as p varies, for different (fixed) values of t. This is a family of straight lines. In Figs. 3(a) (for $\delta = 1$) and 3(b) (for $\delta = 2$) (see also the corresponding contour plots of G^{q} in Fig. 2), these lines are drawn for times before, during, and after the collision, and for p between $p_c - 3\hbar/\delta$ and $p_c + 3\hbar/\delta$. Note that before the collision (bottom line), $\eta = 1$, and after the collision (top line), $\eta \simeq 0$, because the transition from p to $-p$ has been completed, whereas η can take on large positive values during the collision (middle line). The value of p where $G^{\mathrm{q}}(p,t)$ is maximum, for a given value of time, can be read from the cut between the line $z_+(p)$ (for $p > p_c$) and the contour level $\log_{10}(\eta) = 0$. This is the point where the two distributions coincide; see

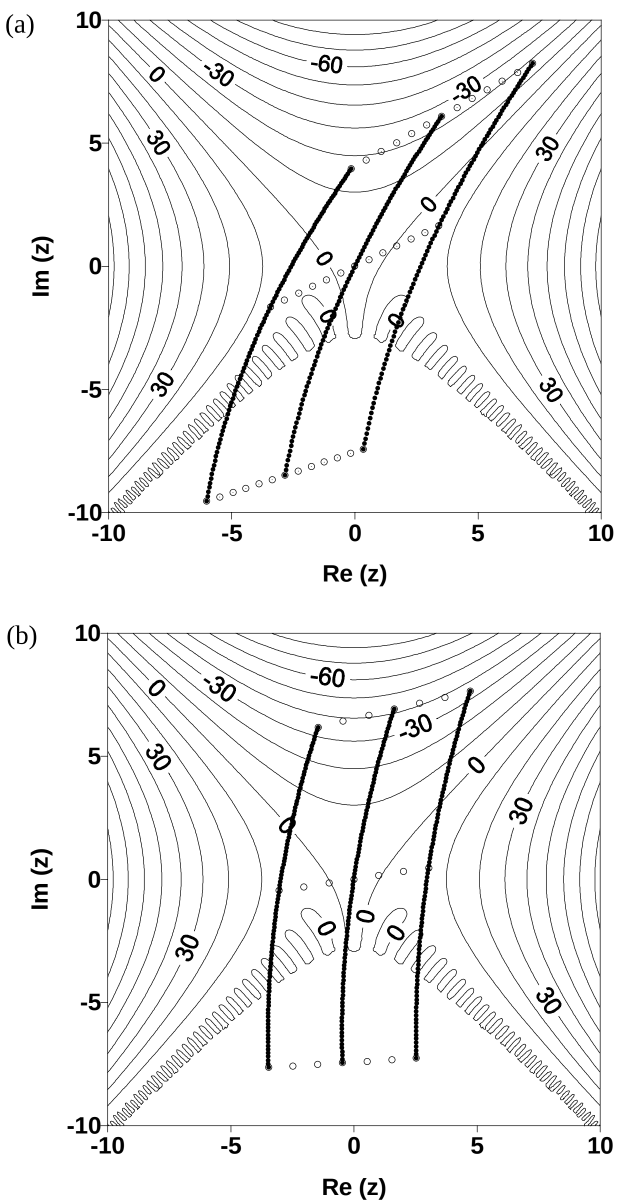

FIG. 3. Contour plot of $\log_{10}[\eta(z)]$. Three curves $z_+(t)$ for $p = p_c - 3\hbar/\delta$ (left), $p = p_c$ (middle), and $p = p_c + 3\hbar/\delta$ (right) are represented by solid circles for the wave packet (8) with $p_c = 20$, $x_c = -50$ and (a) $\delta = 1$ or (b) $\delta = 2$. Empty circles represent $z_+(p)$ for times before collision (bottom), $t = 2.5$ (middle), and after collision (top). The circles are drawn every $\Delta p = 0.5$.

also Fig. 1. The maximum is shifted to lower momenta when δ increases, as confirmed in Fig. 2.

Alternatively, z_+ can be drawn as t varies, for fixed values of p. Figures 3(a) and 3(b) show curves $z_+(t)$ for $p = p_c$ and $p = p_c \pm 3\hbar/\delta$. The latter "explore" regions of the z plane where η is larger than for the central momentum.

The presence of w functions (and related "complementary error functions" or "Moshinsky functions" [3]) is by no means a peculiarity of this model. In fact these functions may be considered as the elementary propagators of the Schrödinger transient modes [4], and therefore the type of analysis just performed can be extended to more complex cases [5,6].

This momentum enhancement is not related to certain effects that involve "anomalously high velocities." In recent years there has been much discussion and controversy about the propagation of evanescent waves. Measurements of "superluminal" velocities have been reported for photons [7], and similar effects were predicted and studied for particles in collisions involving tunneling across opaque barriers by Hartman [8]. The Hartman effect can be described by considering only the asymptotic regimes (before and after the collision) and comparing average passage times for the incident wave packet with the actual transmitted wave packet [9,10]. The latter is advanced (in particular its peak) with respect to the former, but no enhancement of the momentum distribution similar to the one depicted in Fig. 1 takes place asymptotically. The effect described in this Letter and the anomalously high velocities reported in evanescent wave conditions are not connected to each other (although trying to find a possible link was our original motivation). The enhancement effect is universal and does not require evanescent conditions. A second asymptotic effect also unrelated to the one discussed in this Letter is the acceleration that the transmitted wave packet suffers because of the "filtering" of the potential barrier. The transmission coefficient $|T(p)|^2$ favors the passage of higher momentum components so that the average of the momentum distribution of the transmitted packet is usually shifted to larger values than the original one. However, because of the asymptotic kinetic energy conservation, Eq. (5), the momentum distribution itself $|\psi(p,t)|^2$, cannot exceed the original curve $|\psi(p,0)|^2$.

In spite of being a transient effect, the enhancement of high momenta is in principle measurable, for example, by suddenly switching the potential off during the collision and analyzing the resulting momentum distribution as in Ref. [11]. In the sudden limit, the momentum distribution remains unaltered by the change of the Hamiltonian, from t_0 to t_1 [12]. The condition of validity of the sudden approximation is $T \ll \hbar/\Delta\overline{H}$, where $T \equiv t_1 - t_0$ is the switching time, $\overline{H}$ is the time average of the Hamiltonian during the interval (t_0, t_1), and $\Delta\overline{H}$ is calculated for the state of the system at t_0 [12]. The experiment may be implemented with ultracold atoms colliding with a potential barrier created by a laser beam [13,14]. The switching times (~ 0.5 μs) and atomic velocities ($\sim$mm/s) recently achieved would allow one to satisfy the above condition.

We acknowledge A. M. Steinberg for useful discussions about the possible experimental verification of the effect. Support from Gobierno de Canarias (Grant No. PI2/95) is also acknowledged.

[1] A principal part is always present in the momentum representation of the scattered wave of the Lippmann-Schwinger equation, which is the basic framework for all scattering processes, regardless of the dimensionality.
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