

A quantum evaporation effect

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Abstract. – A small momentum transfer to a particle interacting with a steep potential barrier gives rise to a *quantum evaporation* effect which increases the transmission appreciably. This effect results from the unexpectedly large population of quantum states with energies above the height of the barrier. Its characteristic properties are studied and an example of physical system in which it may be observed is given.

It is well known that the wave nature of quantum motion can amplify as well as reduce quantum transport in comparison with its classical counterpart. For example, a quantum particle is able to tunnel through a potential barrier, a behaviour which is, of course, not possible in classical mechanics. On the contrary, the same particle is very likely to move in a certain part only of a random medium [1] whereas a classical particle may wander through the whole of it. The Schrödinger equation leads therefore to a large variety of situations regarding transport, whose study is still the subject of active research (see, *e.g.*, [2–4]).

In this letter, we describe a novel effect, called *quantum evaporation* hereafter, in which the wave nature of quantum motion amplifies transport appreciably. We study the behaviour in one dimension of a particle which undergoes a small momentum transfer while interacting with a rectangular potential barrier or with a potential step, both of height larger than its kinetic energy. We first present wave packet simulations of this behaviour, which reveal that a small momentum transfer is able to produce a large increase of the transmission into the classically forbidden region. We then explain this increase by relating it to the population, induced by the momentum transfer, of the quantum states with energies above the height of the potential. The population of these quantum states enables the particle to move in the classically inaccessible region, and so gives rise to quantum evaporation. We finally give an example of physical system in which this effect could be observed.

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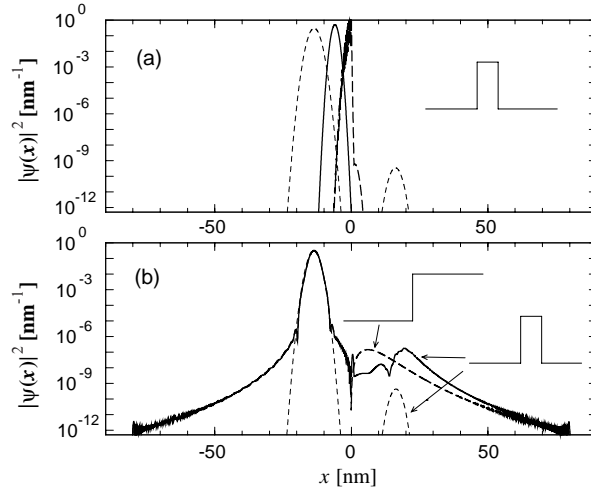


Fig. 1 – Effect of a momentum transfer on the propagation of a wave packet $\psi(x)$. a) *Without momentum transfer*. At $t = 0$ s, a wave packet of Gaussian shape is sent towards a potential barrier (solid line). At $t \simeq 4.5 \times 10^{-15}$ s, the centroid of the wave packet reaches the potential barrier (long-dashed line). At $t \simeq 15 \times 10^{-15}$ s, the transmitted and reflected wave packets are well separated (dashed line). b) *With a momentum transfer*. The shapes of the reflected and transmitted wave packets are plotted at $t \simeq 15 \times 10^{-15}$ s. Dashed line: transfer at $t = 0$ s and potential barrier. Solid line: transfer at $t \simeq 4.5 \times 10^{-15}$ s and potential barrier. Long-dashed line: transfer at $t \simeq 4.5 \times 10^{-15}$ s and potential step. See text for details.

Figure 1 shows the shape of a quasi-monochromatic wave packet at a few given times of its interaction with a potential⁽¹⁾. This wave packet has an initial shape which is Gaussian, with the centroid at the position $x_i = -6$ nm and the standard deviation $\sigma = 0.8$ nm. Its initial wave number distribution is centred on the average wave number $\bar{k} \simeq 1.2 \times 10^{10} \text{ m}^{-1}$ and has the standard deviation $\delta k = 1/(2\sigma) \simeq 0.05\bar{k}$. In addition, the wave packet has an average initial kinetic energy $E_i = \hbar^2 \bar{k}^2 / (2m) = 5$ eV (m is the mass of the particle), a typical energy for an electron in a metal. In fig. 1a, it interacts with a rectangular potential barrier of height $V_0 = 10$ eV which extends from $x = 0$ to $x = 1$ nm, a typical barrier in solid state physics. The resulting transmission probability, $T \simeq 1.2 \times 10^{-9}$, is of the same order of magnitude as the transmission probability $T \simeq 4.5 \times 10^{-10}$ for a purely monochromatic wave. It is much larger than the classical probability to have an energy larger than V_0 , which is only $0.5 \operatorname{erfc}((\sqrt{mV_0}/\hbar - \bar{k}/\sqrt{2})/\delta k) \simeq 0.7 \times 10^{-15}$.

In fig. 1b, the wave packet undergoes a small instantaneous momentum transfer $\hbar q$, with $q = 10^8 \text{ m}^{-1} \simeq 10^{-2}\bar{k}$. If the transfer occurs at time $t = 0$ s (dashed line), *i.e.* much before the time $t_0 = m|x_i|/(\hbar\bar{k}) \simeq 4.5 \times 10^{-15}$ s at which the centroid of the wave packet reaches the potential, the transmission probability increases only slightly, reaching the value $T \simeq 1.5 \times 10^{-9}$. This is in agreement with the related small increase of the average kinetic energy from $E_i = 5$ eV to $E_f = \hbar^2(\bar{k} + q)^2 / (2m) \simeq 5.09$ eV. On the contrary, if the transfer

⁽¹⁾The evolution of the wave packet is obtained by numerical integration of the time-dependent Schrödinger equation according to the standard Crank-Nicholson method [5]. Grid spacings of 2.5×10^{-18} s in time and 1.5×10^{-12} m in space have been used in our calculations. The resulting accuracy on the values of the transmission probability T is better than 3%. Note that the results of our wave packet simulations are quite general because they can be adapted to any quantum particle with the help of the usual scaling relations of the Schrödinger equation for time, length and wave number.

happens at a time very close to t_0 (solid line), the transmission probability increases up to $T \simeq 1.1 \times 10^{-6}$. Such a large increase of the transmission probability, whose study is the subject of this letter, can no longer be explained by the variation of the average kinetic energy. The shape of the transmitted wave packet, plotted at time $t \simeq 15 \times 10^{-15}$ s, is no longer Gaussian whereas it is still nearly so in the case of the transfer at $t = 0$ s.

Figure 1b shows also the shape of the wave packet in the case of a potential step $V(x) = V_0 H(x)$ ($H(x)$ is the Heaviside function) and of the momentum transfer at a time $t \simeq t_0$ (long-dashed line). In the region $x > 1$ nm, the transmitted wave packet is unexpectedly similar to the one in the case of the potential barrier. As time progresses, it propagates in the classically forbidden region $x > 0$, a behaviour which would hardly be possible with a momentum transfer taking place much before the time t_0 . The corresponding transmission probability, $T \simeq 1.4 \times 10^{-6}$, has nearly the same value as in the case of the potential barrier. These observations together with the preceding ones inevitably lead to the following conclusion. A small momentum transfer which comes about while the centroid of the wave packet is close enough to the potential populates the quantum states with energies above V_0 , even though the average final kinetic energy is less than V_0 . The population of these states is then responsible for the large increase of the transmission probability observed in the wave packet simulations. Thus, in spite of being of negligible weight in the wave packet before momentum transfer, the quantum states with energies above V_0 do play a crucial role after the momentum transfer has happened.

In order to identify the origin of the observed effect, we have examined more precisely the influence of the *time* at which the momentum transfer takes place. Figure 2 shows that the transmission probability T depends approximately as a Gaussian $T_{\max} \exp[-(t - t_0)^2/2(\Delta t)^2]$ on the time t of occurrence of the momentum transfer. The time at which the transmission probability takes its largest value $T_{\max} \simeq 1.4 \times 10^{-6}$ is precisely the time $t_0 \simeq 4.5 \times 10^{-15}$ s at which the centroid of the wave packet reaches the potential step. The length $2\Delta t \simeq 1.2 \times 10^{-15}$ s of the time interval within which the momentum transfer must take place to produce a large increase of the transmission is found to be nearly equal to the duration $2m\sigma/(\hbar k)$ of appreciable interaction of the wave packet with the potential. If the momentum transfer comes about at a time $t \ll t_0 - \Delta t$, *i.e.* much *before* the interaction of the wave packet with the potential, it shifts the initial wave number distribution without reshaping it (see fig. 1b, dashed line). The quantum states with energies above V_0 are then scantily populated and the resulting transmission is small. On the contrary, if the momentum transfer happens within the interval $t_0 - \Delta t \leq t \leq t_0 + \Delta t$, *i.e.* *during* the interaction of the wave packet with the potential, it modifies largely the initial wave number distribution (see fig. 1b, solid and long-dashed lines). The quantum states with energies above V_0 are then well populated and the resulting transmission is large.

We have also studied the influence of the *duration* δt of the momentum transfer. A non-instantaneous transfer is found to produce the same increase of the transmission as an instantaneous one, provided that it is fast enough (*i.e.* $\delta t \leq 10^{-16}$ s). Thus, we focus only on instantaneous momentum transfers in the sequel. It should be noted that the observed effect is *not* interpretable as a trivial consequence of a (naively applied) time-energy uncertainty relation. Indeed, the energy spread $\delta E = \hbar/\delta t$ which is supposed to correspond to $\delta t = 10^{-16}$ s would be of the order of V_0 . It would therefore give rise to a transmission of order unity, which is obviously incompatible with our results. As shown below, the energy distribution after momentum transfer does definitely not result from a time-energy uncertainty relation.

In order to find the characteristic properties of the observed increase of the transmission, we use the following model. Our initial wave packet includes only eigenfunctions $\psi_k(x)$ of the Hamiltonian describing the motion of the particle in the presence of the potential which have

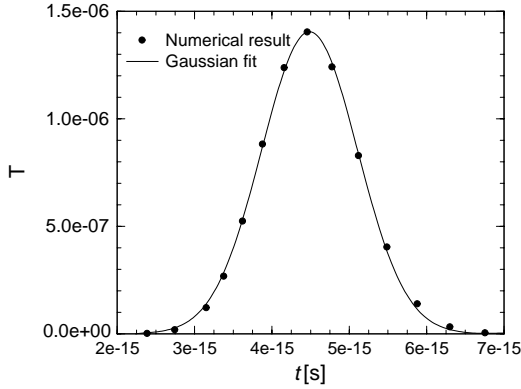


Fig. 2

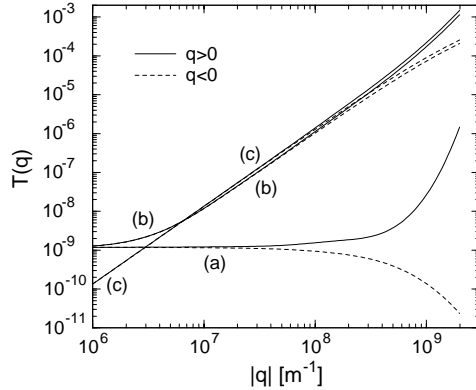


Fig. 3

Fig. 2 – Variation of the transmission probability T with the time t of occurrence of the momentum transfer in the case of the potential step. All parameters as in fig. 1.

Fig. 3 – Variation of the transmission probability T with the transferred wave number q . Wave packet and potential parameters as in fig. 1 ($\bar{k} \simeq 1.2 \times 10^{10} \text{ m}^{-1}$). (a) Transfer *before* interaction with the potential barrier. (b) Transfer *during* the interaction with the potential barrier. (c) Transfer *during* the interaction with the potential step.

an energy below V_0 . In the case of the potential step, the expression of these eigenfunctions is ($0 \leq k < \kappa_0 = \sqrt{2mV_0}/\hbar$)

$$\begin{aligned} \psi_k(x) = & \frac{1}{\sqrt{2\pi}}(1 - H(x)) \left(e^{ikx} + \frac{k - i\sqrt{\kappa_0^2 - k^2}}{k + i\sqrt{\kappa_0^2 - k^2}} e^{-ikx} \right) + \\ & + \frac{1}{\sqrt{2\pi}} H(x) \frac{2k}{k + i\sqrt{\kappa_0^2 - k^2}} e^{-\sqrt{\kappa_0^2 - k^2}x}. \end{aligned} \quad (1)$$

We take here the potential step in preference to the potential barrier so as to emphasize the fact that the studied effect is genuinely different from tunnelling⁽²⁾. The transfer of a momentum $\hbar q$ is modelled by a quantum jump, as in the stochastic wave function description of the evolution of open quantum systems [6]. This quantum jump induces a translation in momentum space of every eigenfunction in the wave packet, *i.e.* $\psi_k(p) \rightarrow \psi_k(p - \hbar q) = \psi_{k,q}(p)$. The expression of the wave function $\psi_{k,q}(x)$ which corresponds to a given eigenfunction $\psi_k(x)$ in the wave packet and takes the effect of the momentum transfer into account is then readily obtained by a Fourier transformation of the translated wave function $\psi_k(p - \hbar q)$. It is

$$\psi_{k,q}(x) = e^{iqx} \psi_k(x). \quad (2)$$

We restrict ourselves to the case of small momentum transfers, characterized by the condition $\hbar^2(k + q)^2/(2m) < V_0$. This condition ensures, of course, that any transmission produced by a momentum transfer cannot be due to a trivial increase of the kinetic energy above V_0 .

The existence of a position-dependent phase factor on the right-hand side of eq. (2) has the striking consequence that a wave function $\psi_{k,q}(x)$ is no longer an eigenfunction of the

⁽²⁾The results of this letter are in fact valid for any potential whose slope on the side where the particle comes in varies rapidly over a de Broglie wavelength. Generally speaking, the steeper the slope, the larger the transmission due to quantum evaporation.

Hamiltonian describing the motion of the particle in the presence of the potential. Hence, $\psi_{k,q}(x)$ may be expanded in terms of the eigenfunctions of this Hamiltonian, *i.e.*

$$\psi_{k,q}(x) = \int_0^{\kappa_0} dk' C_{k'}^k(q) \psi_{k'}(x) + \int_{\kappa_0}^{+\infty} dk' (C_{-k'}^k(q) \psi_{-k'}(x) + C_{k'}^k(q) \psi_{k'}(x)) , \quad (3)$$

with $C_{k',-k'}^k(q) = \int_{-\infty}^{+\infty} dx \psi_{k',-k'}^*(x) \psi_{k,q}(x)$. The first integral in this expansion includes the nondegenerate eigenfunctions with energies below V_0 (cf. eq. (1)) and the second one the doubly degenerate eigenfunctions with energies above V_0 ($|k'| > \kappa_0$). Because of the eigenfunctions with energies above V_0 , every wave function $\psi_{k,q}(x)$ has components which are free to propagate anywhere in space, thus giving rise to a finite probability of quantum evaporation into the classically inaccessible region $x > 0$.

If $f(k)$ denotes the amplitude corresponding to the initial wave number distribution, the time-dependent wave packet which takes the effect of the momentum transfer into account is $\int_0^{\kappa_0} dk f(k) \psi_{k,q}(x, t)$. The probability $T(q)$ of transmission into the classically forbidden region is then defined through the relation $T(q) = \lim_{t \rightarrow +\infty} \int_0^{+\infty} dx \left| \int_0^{\kappa_0} dk f(k) \psi_{k,q}(x, t) \right|^2$. A close study of the wave packet simulations shows that $T(q)$ is dominated by the contributions with energies above V_0 . The transmission probability may therefore be computed accurately with the help of the following formula:

$$T(q) \sim \lim_{t \rightarrow +\infty} \int_0^{+\infty} dx \left| \int_0^{\kappa_0} dk f(k) \int_{\kappa_0}^{+\infty} dk' e^{-\frac{i\hbar k'^2}{2m}t} (C_{-k'}^k(q) \psi_{-k'}(x) + C_{k'}^k(q) \psi_{k'}(x)) \right|^2 . \quad (4)$$

A tedious yet straightforward calculation using the expressions of the wave functions $\psi_{k,q}(x)$ and of the eigenfunctions $\{\psi_{k'}(x), \psi_{-k'}(x)\}$ with energies above V_0 leads to the following formulae for the amplitudes $C_{-k'}^k(q)$ and $C_{k'}^k(q)$ in eq. (4):

$$\begin{aligned} C_{-k'}^k(q) &= \frac{4i\kappa_0^2 k \sqrt{k'^2 - \kappa_0^2}}{\pi \left(k' + \sqrt{k'^2 - \kappa_0^2} \right) \left(k + i\sqrt{\kappa_0^2 - k^2} \right)} \times \\ &\times \frac{q}{((k' + q)^2 - k^2)} \frac{1}{\left(\sqrt{\kappa_0^2 - k^2} - iq \right)^2 + k'^2 - \kappa_0^2} , \end{aligned} \quad (5)$$

$$\begin{aligned} C_{k'}^k(q) &= \frac{4i\kappa_0^2 k k'}{\pi \left(k' + \sqrt{k'^2 - \kappa_0^2} \right) \left(k + i\sqrt{\kappa_0^2 - k^2} \right)} \times \\ &\times \frac{q}{(k'^2 - (k + q)^2)(k'^2 - (k - q)^2)} \frac{\left(\sqrt{\kappa_0^2 - k^2} + i\sqrt{k'^2 - \kappa_0^2} + iq \right)}{\left(\sqrt{\kappa_0^2 - k^2} + i\sqrt{k'^2 - \kappa_0^2} - iq \right)} . \end{aligned} \quad (6)$$

A first notable property of quantum evaporation follows directly from the expressions of the amplitudes $C_{-k'}^k(q)$ and $C_{k'}^k(q)$. Equations (5) and (6) show that both amplitudes are ratios of products of algebraic functions of the wave numbers k , k' and q . Consequently, the effect of quantum evaporation decreases only *algebraically* in k' if this wave number increases from κ_0 up to infinity. This algebraic decrease explains why quantum evaporation produces much larger transmissions than tunnelling does (whose effect decreases *exponentially* in $\sqrt{\kappa_0^2 - k^2}$ if this wave number increases from zero up to κ_0), as one can see by comparing the curves (b) and (c) to the curves (a) in fig. 3.

Since quantum evaporation has a large effect on the transmission, it is interesting to examine the magnitude of the energy transfers. The average energy E_f of the particle after momentum transfer is [7]

$$E_f = \hbar^2(\overline{k^2} + q^2)/(2m) < V_0. \quad (7)$$

Thus, for small momentum transfers $\hbar q$ such that $|q| \ll \overline{k}$, the energy transfer $E_f - E_i = \hbar^2 q^2/(2m)$ is negligible in comparison with the average initial energy E_i . This point reveals another remarkable property of quantum evaporation, namely that an appreciable increase of the transmission does not require a large variation of the average energy. This is so because the multiplication of any $\psi_k(x)$ by a factor e^{iqx} (cf. eq. (2)) removes the stationary character of this wave function, and so increases the transmission, irrespective of the magnitude of the transferred wave number q . The smallness of the variation of the average energy comes from the fact that the momentum transfer populates states with energies above as well as below E_i . It should be noted that a small momentum transfer *before* the interaction of the wave packet with the potential produces an average energy transfer $E_f - E_i = \hbar^2((\overline{k+q})^2 - \overline{k^2})/(2m) \simeq \hbar^2 \overline{k} q/m$. Interestingly enough, this average energy transfer is far larger than the previous one, even though the resulting transmission is much smaller than in the case of quantum evaporation.

The amplitudes $C_{-k'}^k(q)$, eq. (5), and $C_{k'}^k(q)$, eq. (6), are proportional to the transferred wave number q in the regime $|q| \ll (\kappa_0^2 - k^2)/(2\kappa_0)$ [7]. The transmission probability, eq. (4), has then the following simple expression:

$$T(q) \propto q^2. \quad (8)$$

Therefore, whether the particle undergoes a forward ($q > 0$) or backward ($q < 0$) momentum transfer, the resulting transmission increases by the same amount if $|q| \ll (\kappa_0^2 - k^2)/(2\kappa_0)$. This insensitivity to the sign of q is a third characteristic property of quantum evaporation. It can be understood by remembering that the multiplication of any $\psi_k(x)$ by a factor e^{iqx} (cf. eq. (2)) removes the stationary character of this wave function, and so increases the transmission, irrespective of the sign of the transferred wave number q . By comparison, the effect of a momentum transfer coming about *before* the interaction of the wave packet with the potential amounts merely to a trivial shift in momentum, and the resulting transmission then increases or decreases according to whether q is positive or negative.

Figure 3 shows the variation of the transmission probability T with the transferred wave number q for the cases considered in fig. 1b. In the case of a momentum transfer *before* the interaction with the potential barrier (curves (a)), the variation of $T(q)$ is small and depends on the sign of q because the transmission is mainly due to tunnelling. On the contrary, in the case of a momentum transfer *during* the interaction with the potential barrier (curves (b)), $T(q)$ increases by several orders of magnitude because the transmission is fully dominated by quantum evaporation. For any value of q in the regime $|q| \ll (\kappa_0^2 - k^2)/(2\kappa_0)$, $T(q)$ is independent of the sign of q and varies quadratically (up to $|q| \simeq 0.02\overline{k}$), in agreement with eq. (8). The energy transfer becomes of course important at larger values of q , with the expected consequence that a forward momentum transfer produces a larger transmission than a backward one does. In the case of a momentum transfer *during* the interaction with the potential step (curves (c)), the transmission is of course caused by quantum evaporation only. The corresponding curves are nearly identical to the curves (b), which confirms the fact that tunnelling has a negligible effect on the transmission in the case of the potential barrier.

Finally, we would like to point out that there are physical systems which may be used to detect the existence of quantum evaporation. For instance, systems in which electrons are field emitted from a metal surface upon the application of a strong electric field could

be employed with this aim in view. In such systems, quantum evaporation could result from electron-electron or electron-phonon scattering events taking place in the metallic tip. It would then lead to the appearance of a high-energy tail with a tell-tale shape in the spectrum of field-emitted electrons [8]. Laser-cooled atomic gases should prove to be even more interesting for the observation of the effect. This is so because, by switching a resonant laser beam on and off, one controls both the value and the time of occurrence of a momentum transfer to any such system. We have considered a numerical example in which cold metastable helium atoms are sent with an average initial kinetic energy of 10^{-11} eV towards a potential step whose mean height is equal to 1.5×10^{-11} eV. Owing to recent advances in the field of laser cooling techniques, kinetic energies of such small values are now reachable in practice [9]. The corresponding de Broglie wavelengths are then sufficiently large for a potential step with a steep enough slope to be generated (cf. footnote ⁽²⁾). Since the duration of interaction of a cold helium atom with the potential is of the order of 10^{-3} s, one has ample time to create a momentum transfer by spontaneous emission of a photon. This can be done in practice by adjusting, for instance, the laser to the transition $2^3S_1 \rightarrow 2^3P_1$ (lifetime of $2^3P_1 \simeq 100$ ns). Our calculations indicate that a backward wave number transfer of $q = -5 \times 10^5 \text{ m}^{-1}$ (which corresponds to an energy transfer of 1.3×10^{-12} eV) increases the transmission probability from less than 10^{-10} up to 5×10^{-4} , thus producing a potentially detectable effect. Lastly, let us mention that one may also obtain a quantum evaporation effect by giving a velocity $v = \hbar q/m$ to the potential instead of transferring a momentum $\hbar q$ to the atoms, as can be shown by using a Galilean transformation of the Schrödinger equation [7].

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