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A new phase time formula for opaque barrier tunneling

Stefano De Leo and Vinicius Leonardi

Department of Applied Mathematics, State University of Campinas, SP 13083-970, Campinas, Brazil

E-mail: deleo@ime.unicamp.br

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Abstract

After a brief review of the derivation of the standard phase time formula, based on the use of the stationary phase method, we propose, in the opaque limit, an alternative method to calculate the phase time. The *new* formula for the phase time is in excellent agreement with the numerical simulations and shows that for wave packets, whose upper limit of the momentum distribution is very close to the barrier height, the transit time is *proportional* to the barrier width.

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1. Introduction

The time spent by a particle to tunnel across a barrier surely represents one of the most intriguing and challenging discussions found in the literature. After the stimulating articles by MacColl [1] and Hartman [2] on the dynamics of the wave packet which tunnels potential barriers, many tunneling time definitions have been introduced and paradoxical effects, such as superluminal velocities, discussed. Of special interest to us is the discussion on the time spent by non-relativistic particles to cross the classical forbidden region. The extensive literature on tunneling times is reviewed in many reports. For a detailed discussion on phase, dwell and Larmor times, we refer the reader to the report by Hauge and Stovneng [3], for photon and particle tunneling reviewed by a unified time analysis to the report by Olkhovsky, Recami and Jakiel [4], and, finally, for a clear, comprehensive and complete discussion of the tunneling time definitions, paradoxes and proposed solutions to the excellent work by Winful [5]. In this report, it is also found a challenging electromagnetic analogy with the frustrated total internal reflection and resonant tunneling.

In this paper, we present a detailed analytic and numerical analysis of the phase time for non-relativistic wave packets which tunnel opaque barriers. In the opaque limit, due to the filter effect, approximations on the transmission coefficient allow us to find a closed formula for the time in which the peak of the transmitted wave appears in the free region after the barrier.

The *new* formula, which generalizes the well-known formula obtained by the stationary phase method, shows that, for momentum distributions whose upper limit is very close to the barrier height, the phase time is *proportional* to the barrier width. The study is carried out for a potential barrier V_0 with discontinuity in $x = 0$ and $x = L$.

The method commonly used in calculating the transmitted amplitude is based on solving, separately, the Schrödinger equation for stationary states within the potential region and in the free regions before and after the barrier and, then, imposing the continuity of the wavefunction and its derivative at the discontinuities of the potential. After simple algebraic computations, we find the following transmitted amplitude [5, 6]:

$$T(k) = \mathrm{e}^{-\mathrm{i}kL} \bigg/ \left[\cosh(qL) - \mathrm{i}\frac{2k^2 - w^2}{2kq}\sinh(qL)\right], \tag{1}$$

where $q = \sqrt{w^2 - k^2}$ and $w = \sqrt{2mV_0}/\hbar$. The resultant transmitted wave packet is obtained by integrating over all the possible stationary states modulated by a weighting function $g(k)$,

$$\Phi_T(x,t) = N \int_0^{k_M} \mathrm{d}k\, g(k)\ |T(k)|\ \mathrm{e}^{\mathrm{i}\varphi}\ \mathrm{e}^{\mathrm{i}[k(x-L)-Et/\hbar]}, \tag{2}$$

where $\varphi - kL$, with $\varphi = \arctan[(2k^2 - w^2)\tanh(qL)\,/\,2kq]$ the phase of the transmitted amplitude, $k_M = \sqrt{2mE_M}/\hbar$ the upper limit of the momentum distribution, and N a normalization constant containing the information of the number of incoming electrons. The condition $k_M \leqslant w$ guarantees that the allowed energies are truncated before or at the barrier height V_0. We do not have above barrier contributions and, consequently, only tunneling is responsible for the transmitted wave. We restrict the discussion to pure tunneling, i.e. $E_M \leqslant V_0$, to avoid the phenomenon of multiple diffusion [7, 8].

As is well known [4, 5], the use of the stationary phase method allows us to calculate the time in which the peak of the transmitted wave appears in the free region after the barrier without explicitly solving the integral of equation (2). Unfortunately, this is not sufficient for determining the transit time. In fact, the use of the standard phase time formula requires a careful analysis on the applicability of the stationary phase method. Without such an analysis its indiscriminate use could result in wrong theoretical interpretations on the dynamics of the particle tunneling.

In the next section, we briefly revise the standard derivation of the phase time based on the use of the stationary phase method. Then, in section 3, we obtain, by an analytic study of the transmitted wave, a *new* formula for the phase time. This is done in the opaque limit. The discrepancy between the standard and the new formula for the phase time is clear for E_M close to V_0. To confirm the validity of the new formula, a comparison between analytical results and numerical data is presented in section 4. The agreement is excellent and suggests the use of the new approach proposed in this paper as a new method for estimating the phase time. Our conclusions and possible future investigations are drawn in the final section.

2. Revising the standard phase time formula

The old question of tunneling times is often addressed by studying the phase time through the use of the stationary phase method [9, 10]. This method provides an approximate way to calculate the maximum of an integral. The main idea is that sinusoids with rapidly changing phases will add destructively. This basic principle of asymptotic analysis allows us to find the maximum of an integral independent of the details integrand shape. Such a maximum depends on the derivative of the integrand *phase* calculated at the mean value of the wave number. For the transmitted wave given in equation (2), the phase term is *stationary* for

$$\left[\varphi + k\,(x - L) - \frac{E\,t}{\hbar}\right]'_{\langle k\rangle_T} = 0, \tag{3}$$

where the prime stands for the derivative with respect to k and

$$\langle k\rangle_T = \int_0^{k_M} \mathrm{d}k\, k\, g^2(k)\, |T(k)|^2 \Big/ \int_0^{k_M} \mathrm{d}k\, g^2(k)\, |T(k)|^2. \tag{4}$$

By using equation (3), we find that the phase of the transmitted wave is stationary at $x = L$ for times which satisfy

$$\left\{ \frac{E\,t}{\hbar} - \frac{k\,[w^4 \sinh(2\,qL) + 2\,k^2\,(w^2 - 2\,k^2)\,qL]}{q\,[w^4 \cosh(2\,qL)] + 8\,k^2 q^2 - w^4]} \right\}_{\langle k\rangle_T} = 0. \tag{5}$$

For thin barriers ($k_M L \ll 1$), the modulus of the transmitted coefficient is close to 1. The transmitted wave packet has the same form of the incident packet and, consequently, $\langle k\rangle_T \approx k_0$, where k_0 is the center of the incoming momentum distribution $g(k)$. The phase time is then proportional to L. Observe that for very thin barriers we can always guarantee $q_0 L \ll 1$.

For much thicker barriers ($k_M L \gg 1$), we enter in the so-called opaque limit. In this limit, the peak of the transmitted momentum distribution is shifted to higher wave numbers. This effect is known in the literature as the filter effect [2]. Before beginning our discussion on the phase time formula (5), let us briefly discuss the filter effect. In the opaque limit, the modulus of the transmitted coefficient can be approximated by

$$|\,T(k)\,| \approx 4\,k\,q\,\mathrm{e}^{-q\,L} / w^2. \tag{6}$$

By using this approximation, which also implies $g(k)|T| \approx g(k_M)|T|$, and changing in equation (4) the variable of integration from k to q, we obtain

$$\langle k\rangle_T \approx \int_{q_M}^{w} \mathrm{d}q\, k^2\, q^3\, \mathrm{e}^{-2qL} \Big/ \int_{q_M}^{w} \mathrm{d}q\, k\, q^3\, \mathrm{e}^{-2qL}, \tag{7}$$

where $q_M = \sqrt{w^2 - k_M^2}$. The integrands can now be expanded in series around q_M,

$$k^2 q^3 = k_M^2 q_M^3 + \left(3w^2 - 5q_M^2\right) q_M^2 (q - q_M) + \mathrm{O}[(q - q_M)^2],$$
$$k q^3 = k_M q_M^3 + \left(3w^2 - 4q_M^2\right) q_M^2 (q - q_M)/k_M + \mathrm{O}[(q - q_M)^2].$$

Observing that the main contribution to the integrals in equation (7) comes from the lower limit q_M, we obtain

$$\langle k\rangle_T \approx \frac{k_M^2 q_M + \left(3\,w^2 - 5\,q_M^2\right)/\,2L}{k_M\,q_M + \left(3\,w^2 - 4\,q_M^2\right)/\,2k_M L} \approx k_M - \frac{q_M}{2\,k_M L}\ . \tag{8}$$

The phase of the transmitted wave is then stationary at $x = L$ for times which satisfy

$$\frac{E_M\, t_{\mathrm{Spm}}}{\hbar} \approx \frac{k_M}{q_M}\ . \tag{9}$$

In the next section, we shall propose a new method to calculate the phase time. The *new* phase time formula which reproduces equation (9) for $q_M \sim k_M$ foresees transit times which are proportional to the barrier width L for $q_M \ll k_M$.

3. Proposing a new phase time formula

In the previous section, we estimated the position of the maximum of the transmitted wave packet by using the stationary phase method. In this section, we propose an *alternative* method to calculate the phase time formula. For opaque barrier tunneling, it is possible to calculate explicitly the derivative with respect to the time of the electronic density at the barrier edge and finding when it is equal to zero. This allows us to obtain a *new* formula for the time in which the maximum of the transmitted wave packet is found at $x = L$.

For opaque barrier tunneling, in solving the integral which appears in equation (2), we can use the approximation given in equation (6) and change the variable of integration from k to q. Consequently, the expression of the transmitted wave at the edge of the barrier ($x = L$) becomes

$$\Phi_T(L,t) \approx 4\,N\,g(k_M)\int_{q_M}^{w} \mathrm{d}q\, q^2\,\mathrm{e}^{-qL}\;\mathrm{e}^{\mathrm{i}\,(\varphi - Et/\hbar)}/\,w^2. \tag{10}$$

Due to the filter effect, the phase φ and the energy E can be expanded as follows:

$$\varphi = \varphi_M - 2(q-q_M)/k_M - q_M(q-q_M)^2/k_M^3 + \mathrm{O}[(q-q_M)^3],$$
$$E = E_M - \hbar^2 q_M(q-q_M)/m - \hbar^2(q-q_M)^2/2m.$$

Introducing the new adimensional variable $\rho(q) = (q - q_M)/k_M$ and using the previous expansions, we obtain for the electronic density at $x = L$,

$$|\Phi_T(L,t)|^2 \approx 16|N|^2 k_M^6 g^2(k_M)$$
$$\underbrace{\left|\int_0^{\rho(w)} \mathrm{d}\rho\left(\rho + \frac{q_M}{k_M}\right)^2 \exp\{-\rho k_M L + \mathrm{i}[\alpha(t)\rho + \beta(t)\rho^2]\}\right|^2}_{S(t)} \Big/\, w^4,$$

with

$$\alpha(t) = 2\left(\frac{q_M E_M\,t}{\hbar\,k_M} - 1\right) \quad \text{and} \quad \beta(t) = \frac{E_M\,t}{\hbar} - \frac{q_M}{k_M}\,. \tag{11}$$

The subject matter of this section will be the accurate analysis of $S(t)$ and the calculation of its derivative with respect to time. A first approximation is to consider the first terms in the expansion of the phase time exponential,

$$S(t) \approx |\,s(0) + \mathrm{i}\,[\,\alpha(t)\,s(1) + \beta(t)\,s(2)\,] - \tfrac{1}{2}[\alpha^2(t)s(2) + 2\alpha(t)\beta(t)s(3) + \beta^2(t)s(4)]|^2, \tag{12}$$

where

$$s(n) = \int_0^{\widetilde{w}} \mathrm{d}\rho\left(\rho + \frac{q_M}{k_M}\right)^2 \rho^n \exp[-\rho k_M L] \approx \frac{(n+2)!}{(k_M L)^{n+3}}\left[1 + 2\frac{q_M L}{n+2} + \frac{(q_M L)^2}{(n+2)(n+1)}\right].$$

- The case $q_M \sim k_M$.
  If we limit ourselves to the analysis of processes in which q_M is of the order of k_M, we find that $\beta(t)$ is of the same order of $\alpha(t)$. Observing that in the opaque limit $s(n) \gg s(n+1)$ and that the β-term in $S(t)$ is coupled to $s(n)$ with higher n, we can approximate $S(t)$ as follows:

  $$S(t; q_M \sim k_M) \approx |s(0) + \mathrm{i}\alpha(t)s(1) - \tfrac{1}{2}\alpha^2(t)s(2)|^2 \approx s^2(0) + \alpha^2(t)[s^2(1) - s(0)s(2)].$$

  Deriving $S(t; q_M \sim k_M)$ with respect to time and equating to zero, we obtain $\alpha(t) = 0$. Thus, in this limit, we reproduce the well-known stationary phase condition (9),

  $$S_t(t; q_M \sim k_M) = 0 \quad\Rightarrow\quad \alpha(t) = 0 \quad\Rightarrow\quad \frac{E_M t}{\hbar} = \frac{k_M}{q_M}\,. \tag{13}$$

Table 1. Numerical data for a localized ($d = 20$ Å) non-relativistic ($v_0 = 10^{-3}\,c$) electron with $E_M = V_0$ which tunnels across a barrier potential, $V_0 = 1$ eV. The time in which the transmitted peak appears in the free region after the barrier (second column) is calculated for different values of L. It is clearly the linear dependence on L of the transmission time. Consequently, the barrier transit velocity (third column), defined by L/t, tends to a *constant* value. The ratio between analytical and numerical transit velocities is given in the last column, and shows, as expected, an excellent agreement for increasing values of L.

L $[\hbar/\sqrt{2\,m\,V_0}]$	t $[\hbar/\,V_0]$	v_{tra} $[\sqrt{V_0/\,2\,m}]$	ANA/NUM $\diamond$
50	10.20	4.9013	91.81 %
100	21.41	4.6715	96.33 %
150	32.37	4.6338	97.11 %
200	43.28	4.6209	97.38 %
250	54.17	4.6150	97.51 %
300	65.05	4.6118	97.58 %
350	75.92	4.6099	97.62 %
400	86.79	4.6086	97.64 %
450	97.66	4.6078	97.66 %
500	108.53	4.6072	97.67 %

$\hbar/\sqrt{2mV_0} \approx 2$Å $\hbar/\,V_0 \approx 0.66 \times 10^{-15}s$ $\sqrt{V_0/2m} \approx 10^{-3}c$

- The case $q_M \ll k_M$.
  In this limit, $\alpha \approx -2$ and $\beta(t) \approx V_0 t/\hbar$. The β-term cannot be neglected because for the time of the order of $\hbar L/E_M$ it becomes comparable to the α-term. This implies in our approximation that the terms $s(n)$, $t\,s(n+1)$, and $t^2\,s(n+2)$ are of the same order. Consequently,

$$S(t;\,q_M \ll k_M) \approx \left\{ s(0) - \frac{1}{2}\left[4s(2) - 4s(3)\frac{V_0 t}{\hbar} + s(4)\frac{V_0^2 t^2}{\hbar^2}\right]\right\}^2 + \left[-2s(1) + \frac{V_0 t}{\hbar}s(2)\right]^2$$
$$\approx s^2(0) + 4[s^2(1) - s(0)s(2)] + 4[s(0)s(3) - s(1)s(2)]\frac{V_0 t}{\hbar} + [s^2(2) - s(0)s(4)]\frac{V_0^2 t^2}{\hbar^2}.$$

  By taking the derivative with respect to time and setting it equal to zero, we obtain

$$S_t(t;\,q_M \ll k_M) = 0 \Rightarrow \frac{V_0 t}{\hbar} = \frac{2\,[s(1)s(2) - s(0)s(3)]}{[s^2(2) - s(0)s(4)]} \approx \frac{2\,wL}{9}\ . \tag{14}$$

  The transit velocity, defined as the ratio between the barrier width and the time in which the peak appears in the free region after the barrier, is then given by

$$v_{\text{tra}} = \frac{9}{2}\sqrt{\frac{V_0}{2\,m}}\ . \tag{15}$$

  This analytic result is confirmed by numerical calculations, see table 1. The details of our numerical simulations are found in section 4.

- The general case.
  Observing that for increasing times the terms $\alpha(t)s(n)$, $\beta(t)\,s(n+1)$, and $\beta^2(t)\,s(n+2)$ become comparable, we obtain for $S(t)$ the following expression:

$$S(t) \approx s^2(0) + \alpha^2(t)[s^2(1) - s(0)s(2)] + 2\alpha(t)\beta(t)$$
$$[s(1)s(2) - s(0)s(3)] + \beta^2(t)[s^2(2) - s(0)s(4)\,]. \tag{16}$$

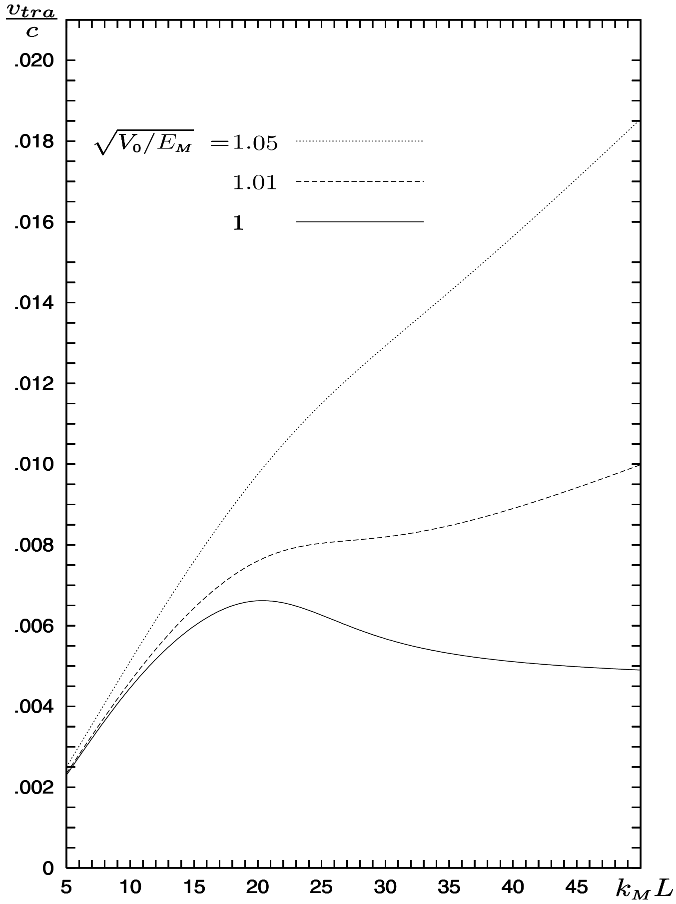

Figure 1. Transit velocities for an incoming (electron) wave packet centered at $k_0 = k_M/2$ with localization determined by $k_M d = 10$ as a function of $k_M L$. For $V_0 \to E_M$, the transit velocity tends to a constant value.

In deriving $S(t)$, we use $\alpha_t(t) = 2\,q_M E_M/\hbar k_M$ and $\beta_t(t) = E_M/\hbar$, and after simple algebraic manipulations, we find

$$\frac{E_M t_{\rm New}}{\hbar} = \frac{2\,(w/k_M)^2\,[s(1)s(2) - s(0)s(3)] + 4\,(q_M/k_M)[s^2(1) - s(0)s(2)]}{[s^2(2) - s(0)s(4)] + 4\,(q_M/k_M)[s(1)s(2) - s(0)s(3)] + 4\,(q_M/k_M)^2[s^2(1) - s(0)s(2)]}. \quad (17)$$

For $q_M \sim k_M$, remembering that in the opaque limit $s(n) \gg s(n+1)$, we find

$$\frac{E_M t_{\rm New}}{\hbar} \approx \frac{4(q_M/k_M)[s(1)s(2) - s(0)s(3)]}{4(q_M/k_M)^2[s^2(1) - s(0)s(2)]} = \frac{q_M}{k_M},$$

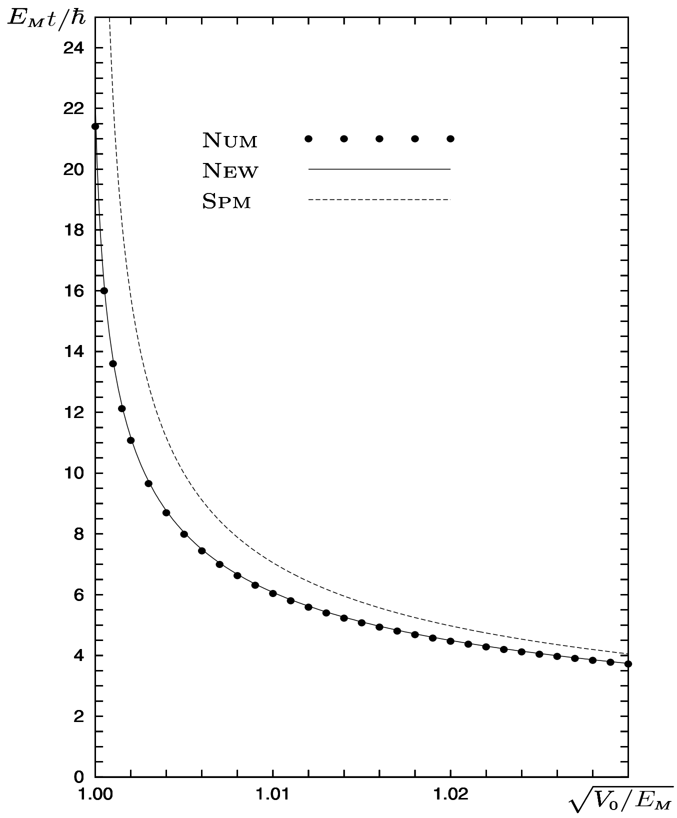

Figure 2. The new phase time formula (NEW), the standard phase time formula obtained by using the stationary phase method (SPM) and the numerical data (NUM) are plotted as the functions of $\sqrt{V_0/E_M}$ for a barrier width determined by $k_M L = 100$. The new phase time formula is in excellent agreement with the numerical analysis. For increasing V_0/E_M, the standard phase time formula represents a good approximation.

as anticipated by equation (13). In the limit $q_M \ll k_M$ the main contribution to the numerator and denominator comes from the first term,

$$\frac{E_M t_{\mathrm{New}}}{\hbar} \approx \frac{2(w/k_M)^2[s(1)s(2) - s(0)s(3)]}{[s^2(2) - s(0)s(4)]} \approx \frac{2[s(1)s(2) - s(0)s(3)]}{[s^2(2) - s(0)s(4)]},$$

reproducing equation (14).

4. Numerical simulations

The *new* phase time formula (17) has been tested for an incoming Gaussian wave packet,

$$g(k) = \begin{cases} \exp[-(k - k_0)^2 d^2/4] & \text{for } 0 \leqslant k \leqslant k_M, \\ 0 & \text{otherwise,} \end{cases}$$

with a localization $d = 10/k_M$, with a momentum distribution centered at $k_0 = k_M/2$, and with an upper limit for the momentum distribution given by $k_M = \text{KeV}/\hbar c$. The incoming electrons move in the free region before the barrier with velocity

$$v_0 = \hbar k_M/2m = \sqrt{E_M/2m} = 10^{-3}c.$$

For a potential barrier of height $V_0 = E_M (= 1\,\text{eV})$, the transit velocity is given, see equation (15), by

$$v_{\text{tra}} = 4.5 \times 10^{-3}c.$$

Numerical data are presented in table 1. The time in which the transmitted peak appears in the free region after the barrier is calculated for different values of L. For increasing L, the transit velocity, v_{tra}, tends to a constant value which is in excellent agreement with the analytic value obtained from equation (15).

To complete our numerical analysis, we have calculated the transit velocity as a function of $k_M L$ for different ratios of V_0/E_M. The plots in figure 1 clearly show that such a velocity tends to a constant value for $V_0 \to E_M$. The standard phase time, the new phase time and the numerical data are plotted in figure 2. The new phase time is in excellent agreement with the numerical simulations. The standard phase time represents a good approximation for increasing values of V_0/E_M.

5. Conclusions

The growing interest in understanding tunneling times in quantum physics stimulated the authors in looking for a new analytic formula of the phase time for wave packets' transmission through opaque barriers. After a brief review of the derivation of the phase time formula, which is based on the stationary phase method, we discuss some intriguing questions about its appropriate use. In the opaque limit, the filter effect is responsible for a shift of the mean value of the transmitted momentum. This allows us to compute directly the transmitted electronic density, and, consequently, by taking the time derivative of this density, to find the time in which the wave packet appears in the free region after the barrier potential. The *new* formula for the phase time is in excellent agreement with the numerical simulations and clearly shows in which cases the standard phase time, calculated by the stationary phase method, represents a good approximation for the transit time. The most important goal of the paper is the proof that, for wave packets whose upper limit of the momentum distribution is very close to the barrier height, the phase time is *proportional* to the barrier width.

Finally, we hope that this work will find readers not only among the physicists interested in tunneling phenomena but also among the specialists in related branches of natural sciences who use the stationary phase method in their practical research.

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