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ABOVE BARRIER POTENTIAL DIFFUSION

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The stationary phase method is applied to diffusion by a potential barrier for an incoming wave packet with energies greater than the height of the barrier. It is observed that a direct application leads to paradoxical results. The correct solution, confirmed by numerical calculations is the creation of multiple peaks as a consequence of multiple reflections. Lessons concerning the use of the stationary phase method are drawn.

Keywords: Quantum mechanics; potential diffusion; stationary phase method.

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The stationary phase method (SPM), first introduced to physics by Stokes and Kelvin,[1] provides an approximate way to calculate the maximum of an integral. It represents a standard calculation tool for physicists, biologists, economists, etc.[2] Below, we shall briefly introduce the method. One of its main attractions is the apparent insignificance of details of the integrand with the exception of its phase. Under its description, a series of limitations and assumptions has been made. While these are known to the experts, they are often assumed implicitly and tested indirectly *a posteriori* by the results obtained.

Recently, much interest in the physics community has been stirred up by the results of this method applied to tunneling times.[3] This has resulted in predictions of super-luminal velocities, or more precisely to tunneling times which, in the so-called opaque limit, are *independent* of the barrier widths[4] and of the distance between the barriers.[5,6] Now, while not addressing this question directly in this paper, we investigate what we consider a simpler but related problem: the (nonrelativistic) diffusion of an incoming single wave packet with energy spectrum completely above the barrier height. We first show that a direct application of the SPM analogous to the tunneling case (energy spectrum below the barrier height) also leads to surprising paradoxical results. We have then performed numerical calculations which clearly display secondary reflected and transmitted peaks. This stimulates the assumption of multiple reflections which, when combined with the SPM, yields excellent agreement with our numerical calculations. The primary lesson that we draw is that the SPM, without additional knowledge such as the number of wave packets existing, is ambiguous and whence meaningless. For diffusion problems the conservation of probabilities can in principle be used to eliminate this ambiguity.

Consider a complex integral over an unspecified range of the form

$$\mathcal{I} = \int F(k)dk = \int |F(k)| \exp[i\theta(k)]dk \,, \tag{1}$$

for which $|F(k)|$ has a single maximum within the range of integration at $k = k_0$. If $\theta(k)$ varies sufficiently smoothly within the interval where $|F(k)|$ is appreciable, we can expand $\theta(k)$ about the point $k = k_0$ in a Taylor series

$$\theta(k) = \theta_0 + (k - k_0)\theta'_0 + O[(k - k_0)^2] \,,$$

where

$$\theta_0 \equiv \theta(k_0) \qquad \text{and} \qquad \theta'_0 \equiv \left.\frac{d\theta(k)}{dk}\right|_{k=k_0} .$$

If the modulus of $F(k)$ is sufficiently sharply peaked, we can neglect the second and higher order terms in the above series. This allow us to approximate the integral in Eq. (1) by

$$\mathcal{I} \approx \exp[i\theta_0] \int |F(k)| \exp[i(k - k_0)\theta'_0]d(k - k_0) \,. \tag{2}$$

If θ'_0 is large, the function of k which is to be integrated oscillates rapidly and, consequently, this integral will be practically null. Thus, a significant contribution only occurs when

$$\theta'_0 = 0 \,. \tag{3}$$

In this study, we consider a modulated plane wave and are interested in the configuration space wave function in one dimension x,

$$\psi(x,t) = \int |F(k)| \exp[i\lambda(k)] \exp[i(kx - Et)]dk \tag{4}$$

with $E = k^2/2m$ (nonrelativistic quantum mechanics). The $F(k)$ may be a Gaussian or similar modulation function. The total phase is

$$\theta(k; x, t) = kx - \frac{k^2}{2m}t + \lambda(k) \,, \tag{5}$$

and the condition $\theta_0' = 0$ then gives the spacetime dependence of the maximum (or peak) of $|\psi(x,t)|$. For example, when $\lambda(k) = 0$ we obtain the group velocity result for a free wave packet, i.e.

$$x = \frac{k_0}{m} t \,. \tag{6}$$

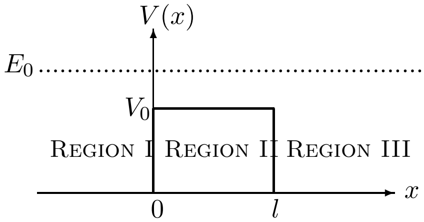
The existence of a $\lambda(k)$ produces a time or space shift,

$$x = \frac{k_0}{m} t - \lambda_0' = \frac{k_0}{m}\left(t - \frac{m\lambda_0'}{k_0}\right) = \frac{k_0}{m}(t - \Delta t) \,.$$

It is exactly this type of analysis which leads to a delay time in the reflection of an incoming wave packet (with momentum or energy spectrum completely below the step height) impacting upon a *step potential*.[7] A similar analysis has been used for tunneling times.[8]

The standard procedure in these (one-dimensional) potential problems is to find the stationary plane wave solutions with the appropriate continuity conditions and then pass to a normalized wave packet by means of a modulating function. While the plane waves exist at all times in an infinite range of x, the wave packet is predicted by the SPM to exist for the incoming wave for say $t < 0$ while the reflected wave and other waves exist only for $t > 0$. Around $t = 0$, we will have interference effects due to the simultaneous presence of both incoming and reflected wave, and for the below barrier case we also have, over this transitory period, a wave function within the classically forbidden barrier region.

In the following figure, we show the potential barrier divided into three regions I ($x < 0$), II ($0 < x < l$) and III ($x > l$). The dotted line indicates the mean energy



$$V(x) = \begin{cases} 0\,, & x < 0 \quad \text{or} \quad x > l\,, \\ V_0\,, & 0 < x < l\,, \end{cases}$$

of the incoming wave,

$$\Psi_{\text{inc}}(x,t) = \int_{\sqrt{2mV_0}}^{\infty} g(k) \exp[i(kx - Et)] dk \,, \tag{7}$$

with $g(k)$ a truncated Gaussian or similar, peaked at k_0 ($E_0 = k_0^2/2m$). Truncation is needed, at least for small k as indicated in Eq. (7) since we wish to avoid any tunneling phenomena. The x-dependence of the plane wave solutions in the three regions are given by

$$\begin{array}{llll} \text{Region I}: & x < 0\,, & \exp[ikx] + R(k)\exp[-ikx] & [k = \sqrt{2mE}]\,, \\ \text{Region II}: & 0 < x < l\,, & A(k)\exp[iqx] + B(k)\exp[-iqx] & [q = \sqrt{2m(E-V_0)}]\,, \\ \text{Region III}: & l < x\,, & T(k)\exp[ikx]\,. & \end{array} \tag{8}$$

$R(k)$ and $T(k)$ are the reflected (region I) and transmitted (region III) amplitudes and the coefficients $A(k)$ and $B(k)$ are the right and left going amplitudes in region II. All the amplitudes are to be modulated by the function $g(k)$. Continuity of $\Psi(x,t)$ and its derivative at $x = 0$ and $x = l$ determines the coefficients A, B, R and T. Explicitly,

$$\begin{aligned} A(k) &= k(k+q)\exp[i\lambda(k) - iql]/\mathcal{D}(k)\,, \\ B(k) &= k(q-k)\exp[i\lambda(k) + iql]/\mathcal{D}(k)\,, \\ R(k) &= (k^2 - q^2)\sin[ql]\exp\left[i\lambda(k) - i\frac{\pi}{2}\right]\Big/\mathcal{D}(k)\,, \\ T(k) &= 2kq\exp[i\lambda(k) - ikl]/\mathcal{D}(k)\,, \end{aligned} \tag{9}$$

where

$$\mathcal{D}(k) = \{4k^2q^2 + (k^2 - q^2)^2\sin^2[ql]\}^{\frac{1}{2}}$$

and

$$\lambda(k) = \arctan\{(k^2 + q^2)\tan[ql]/2kq\}\,.$$

To apply the SPM in what we would call the naive way, we must multiply each of the above amplitudes by the appropriate plane wave phases. For example, in the simplest case of *real* $g(k)$-function, we obtain

$$\theta_{\rm inc}(k) = kx - Et\,, \tag{10}$$

$$\begin{aligned} \theta_R(k) &= \lambda(k) - \frac{\pi}{2} - kx - Et\,, \\ \theta_A(k) &= \lambda(k) + q(x-l) - Et\,, \\ \theta_B(k) &= \lambda(k) + q(l-x) - Et\,, \\ \theta_T(k) &= \lambda(k) + k(x-l) - Et\,. \end{aligned} \tag{11}$$

The presence of the phase term $\lambda(k)$ implies a delay time in the reflected wave analogous to what happens for the step potential when $E < V_0$. Since the phase of the incoming wave contains only the plane wave factors, the incoming peak reaches the barrier at $x = 0$ at time $t = 0$. For the reflected wave, we find the position of the peak at

$$x = \lambda'(k_0) - (k_0/m)t\,, \tag{12}$$

with

$$\lambda'(k_0) = \left[\frac{2}{q}\frac{(k^2+q^2)k^2ql - (k^2-q^2)^2\sin[ql]\cos[ql]}{4k^2q^2 + (k^2-q^2)^2\sin^2[ql]}\right]_{\mathrm{k=k_0}} . \tag{13}$$

Note that only $x < 0$ is physical in this result since the reflected wave, by definition, lies in region I.

The above expression for the position of the reflected peak simplifies around the "resonance" values for k_0 (q_0) where

$$\sin[q_0 l] = 0\,, \quad \text{i.e. } q_0 l = n\pi\,,$$

with n a non-negative integer. Let us assume, for simplicity, a sharp spectrum for $g(k)$ peaked at one of these resonance values,

$$\lambda'_{\mathrm{res}}(k_0) \approx \frac{(k_0^2+q_0^2)l}{2q_0^2} > 0\,. \tag{14}$$

This predicts a delay time for the reflected wave given by

$$\Delta t_R^{\mathrm{res}} = \frac{m}{k_0}\lambda'_{\mathrm{res}}(k_0) \approx \frac{(k_0^2+q_0^2)ml}{2k_0q_0^2}\,. \tag{15}$$

Now consider the corresponding "delay times" for the A, B and T waves. In particular, for the A-wave we find

$$\Delta t_A^{\mathrm{res}} = \frac{m}{k_0}[\lambda'_{\mathrm{res}}(k_0) - q'(k_0)l] = \Delta t_R^{\mathrm{res}} - \frac{m}{q_0}l \approx \frac{(k_0-q_0)^2ml}{2k_0q_0^2}\,. \tag{16}$$

This is the delay time at $x = 0$. We can also calculate a delay time for the B-wave at $x = 0$. However, this time is later than the time at which the B-wave reaches the position $x = l$, this is a consequence of the $q(l-x)$ factor in Eq. (10). Suffice it to say that it arrives at $x = 0$ at a later time than the departure times of either the R or A wave peaks. For completeness the transmitted T wave packet has its peak at the start of region III, $x = l$, at the time

$$t_T^{\mathrm{res}} = t_R^{\mathrm{res}}\,.$$

Now one may be somewhat surprised to note that the appearance of the transmitted wave coincides with that of the reflected wave. However, the above results become paradoxical as soon as one realizes that for the time interval from $t = 0$ to $t = \Delta t_A^{\mathrm{res}} < \Delta t_R^{\mathrm{res}}$ this solution is devoid of *any* maximum (R, A, B or T). During this time, at least, we are clearly in contradiction with probability conservation since the incoming wave peak has disappeared at time $t = 0$. By choosing the wave packet dimensions small enough, we can say that there is an interval of time in which the naive SPM says that there are no significant amplitudes anywhere in x. Note, however, that this is only a heuristic argument since a peaked configuration space packet runs counter to the above resonance approximation (peaked momentum distribution). There are also other incongruities in this naive application of the SPM. If one recalls the well-known step case with $E > V_0$, single peak reflection occurs instantaneously (zero delay time). One might expect that our results tend to this case in the limit $l \to \infty$. This is not the case. It is also possible in some off-resonance cases to find negative "delay times". In these latter cases the maximum of the reflected wave and incoming wave would exist contemporaneously. This situation also implies problems with probability conservation.

Numerical calculations automatically conserve probabilities, at least to within the numerical errors. So to understand what is happening we performed such calculations and an example of these is shown in Fig. 1, where a *complex Gaussian* modulation function

$$g(k) = \left(\frac{a^2}{8\pi^3}\right)^{\frac{1}{4}} \exp\left[-\frac{a^2(k-k_0)^2}{4}\right] \exp[-ikx_0]$$

has been used. It is to be noted that the choice of including a phase factor in $g(k)$ simply shifts all times by a constant mx_0/k_0 at resonance. These figures display the wave function in the *proximity* of the barrier for suitably chosen times. One clearly sees in these figures the appearance of multiple peaks due to the two reflection points at $x = 0$ and $x = l$. This observation suggested the following analysis and imposed the subsequent interpretation.

The R, A, B and T amplitudes may be rewritten as series expansions by considering multiple reflections and transmission in the potential discontinuity points,

$$\begin{aligned} R &= \sum_{n=1}^{\infty} R_n = R_1 + R_2 \left[1 - \left(\frac{k-q}{k+q}\right)^2 \exp[2iql]\right]^{-1}, \\ A &= \sum_{n=1}^{\infty} A_n = A_1 \left[1 - \left(\frac{k-q}{k+q}\right)^2 \exp[2iql]\right]^{-1}, \\ B &= \sum_{n=1}^{\infty} B_n = B_1 \left[1 - \left(\frac{k-q}{k+q}\right)^2 \exp[2iql]\right]^{-1}, \\ T &= \sum_{n=1}^{\infty} T_n = T_1 \left[1 - \left(\frac{k-q}{k+q}\right)^2 \exp[2iql]\right]^{-1}, \end{aligned} \tag{17}$$

with

$$R_1 = \frac{k-q}{k+q}\,, \qquad A_1 = \frac{2k}{k+q}\,, \qquad B_1 = \frac{2k(q-k)}{(k+q)^2} \exp[2iql]\,,$$

$$T_1 = \frac{4kq}{(k+q)^2} \exp[i(q-k)l]\,, \qquad R_2 = \frac{q}{k} A_1 B_1\,, \tag{18}$$

$$\frac{R_{n+2}}{R_{n+1}} = \frac{A_{n+1}}{A_n} = \frac{B_{n+1}}{B_n} = \frac{T_{n+1}}{T_n} = \left(\frac{k-q}{k+q}\right)^2 \exp[2iql] \qquad n = 1, 2, \ldots\,.$$

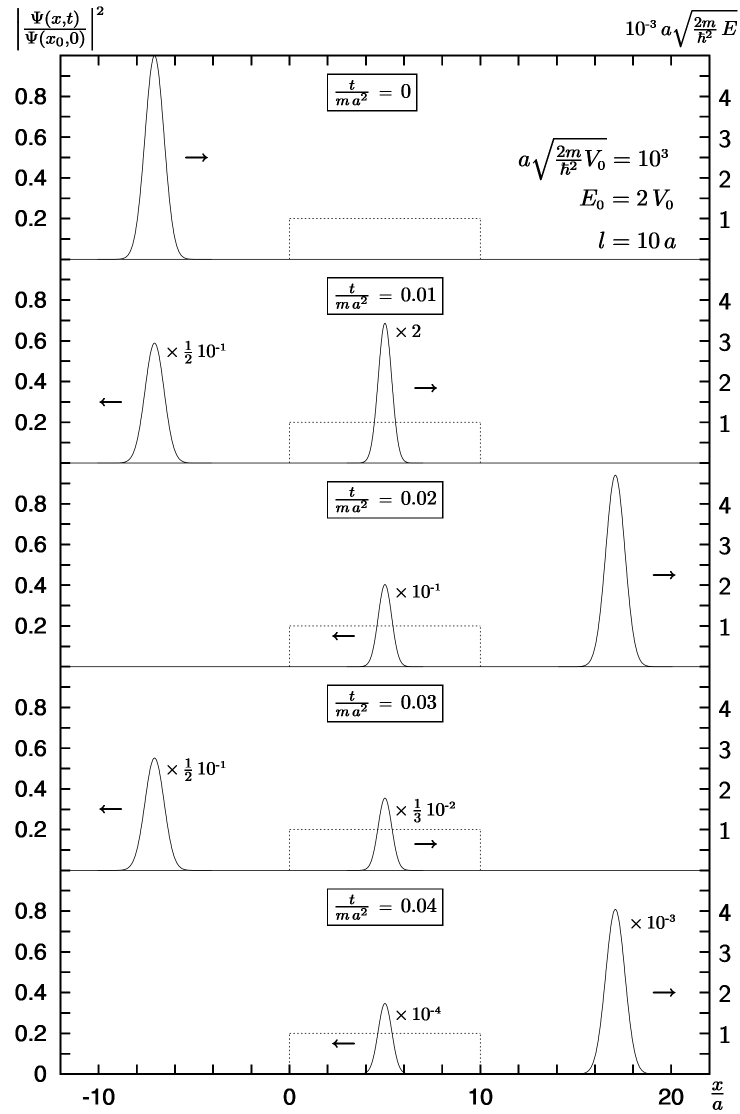


Fig. 1. The square of the amplitude modulus for different time frames. Only a fixed region in x close to the barrier is shown. Each figure should be multiplied by the adjacent factor, where it exists, to obtain the true curve. The parameters chosen for the plot are listed in the first frame.

These sums reproduce exactly the expressions in Eq. (9). In this form the interpretation is easy. R_1 represents the first reflected wave (it has no time delay since it is real). R_2 represents the second reflected wave. As a consequence of continuity, it is the sum, in region II, of the first left-going wave (B_1) and the second right-going amplitude (A_2), i.e.

$$R_2 = A_2 + B_1 \equiv \frac{q}{k} A_1 B_1 \, .$$

This structure is that given by considering two "step functions" back-to-back. Thus at each interface the "reflected" and "transmitted" waves are instantaneous, i.e. without any delay time. Indeed the SPM *applied separately* to each term in the above series expansion for R yields delay times which are integer multiples of $2(dq/dE)_0 l = 2(m/q_0)l$. This agrees perfectly with the fact that since the peak momentum in region II is q_0, the A and B waves have group velocities of q_0/m and hence transit times (one way) of $(m/q_0)l$. The first transmitted peak appears (according to this version of the SPM) after a time $(m/q_0)l$, in perfect agreement with the above interpretation.

Let us re-express what is happening. The incoming wave peak reaches the first potential discontinuity at $x = 0$. It instantaneously yields a first reflected peak (R_1) and right-moving (A_1) peak in region II. When this wave packet reaches at time $t = (m/q_0)l$, the second discontinuity at $x = l$, a part T_1 is transmitted into region III ($x > l$) while a part B_1 is turned back and eventually gives rise to the second reflected peak and so forth. Is this compatible with probability conservation? It is because of the following identity

$$\sum_{n=1}^{\infty}(|R_n|^2 + |T_n|^2) = 1\,. \tag{19}$$

This result is by no means obvious since it coexists with the well-known result, from the plane wave analysis,

$$|R|^2 + |T|^2 = \left|\sum_{n=1}^{\infty} R_n\right|^2 + \left|\sum_{n=1}^{\infty} T_n\right|^2 = 1\,. \tag{20}$$

In Fig. 2 we have re-plotted for various times the numerical calculations displayed in Fig. 1 and also the separate integral calculations based upon the above multiple pole model i.e. for particular $R_n(T_n)$. The latter wave packets are represented by the curves. The former un-decomposed numerical calculations are plotted by various bullets. Agreement is excellent.

In conclusion, the results of the SPM depend critically upon the manipulation of the amplitude prior to the application of the method. *A posteriori* this seems obvious. If we consider an amplitude say

$$z(k; x, t) = |z| \exp[i\alpha]$$

the SPM will yield one peak position for each given time. If we write the identity

$$z = z_1 + z_2\,,$$

where $z_1 = z - w$ and $z_2 = w$, and treat separately these terms, then the same approach will yield two peaks and so forth. The method is inherently ambiguous unless we know, by some other means, at least the number of separate peaks involved. Our above barrier analysis is simply a particular example of this ambiguity, for which we have presented a simple resolution, based upon multiple reflections, confirmed in detail by numerical calculations.

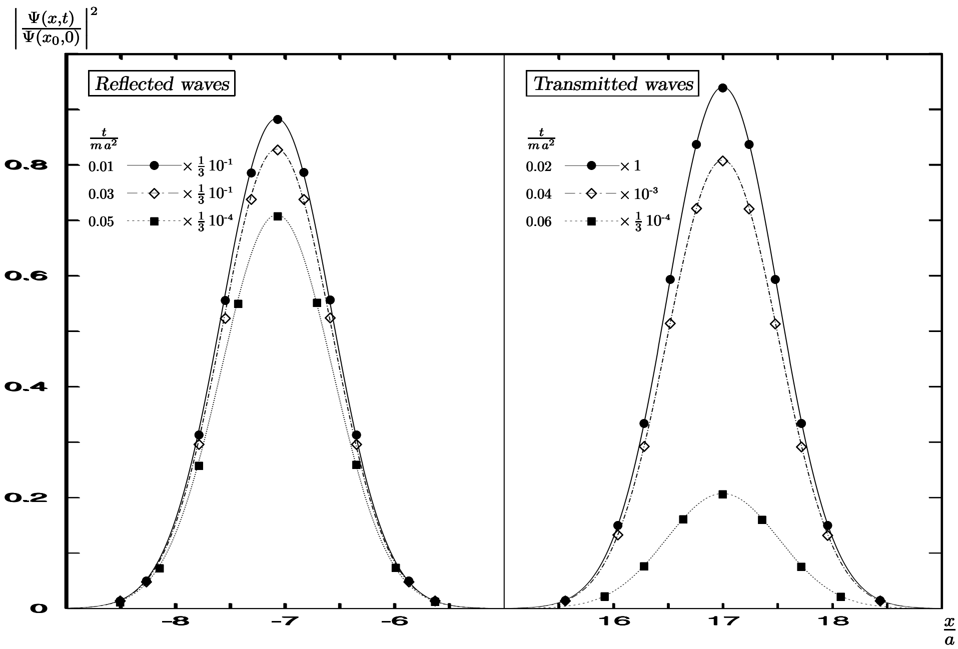


Fig. 2. Plots of the first few reflected and transmitted waves at corresponding times. The bullets are from the numerical convolution of the plane-wave solution. The curves are from the separate convolution integrals of the first three R_n and T_n. Again the true figures are obtained by multiplying by the listed factors.

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