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Uniform solutions for scattering by a potential barrier and bound states of a potential well

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The one-dimensional Schrödinger equation is solved asymptotically for scattering of a particle by a potential barrier and for bound states of a potential well, when the potentials change little in a wavelength. Both solutions are represented uniformly in space, rather than nonuniformly as in the WKB method. This avoids matching expansions and using connection formulas. The scattering solution and the complex reflection and transmission coefficients are also uniform in the particle energy.

I. INTRODUCTION

One-dimensional scattering and bound state problems in quantum mechanics are often solved approximately by the WKB method. This method has an intrinsic defect which makes it inconvenient or difficult to use. It is that different expressions for the solution must be used on each side of a turning point, and they must be matched to a third expression which is valid near the turning point. Thus in a typical bound state or scattering problem with two turning points, five different expressions for the solution must be used and matched to one another.

We shall show how to overcome this defect by using one spatially uniform asymptotic representation of the solution instead of the WKB five-part nonuniform representation. For scattering the spatially uniform representation and the corresponding complex reflection and transmission coefficients are also uniform in the energy of the incident particle. That is, they are valid for the particle energy above, at, or below the peak of the potential. These results are not available in textbooks and they do not appear to be given in the literature either.

To gain these advantages one must use Hermite polynomials for bound state problems and parabolic cylinder functions for scattering problems. Hermite polynomials are already used to treat bound states of a harmonic oscillator, and the present method provides an additional use for them. Parabolic cylinder functions can be used to exactly solve scattering by a parabolic potential barrier, and then used for the approximate solution of scattering by any potential. In fact, in Sec. II we shall treat first the bound states of a harmonic oscillator and then those of a general potential. Similarly, in Sec. III we shall treat scattering by a parabolic potential barrier and then in Sec. IV we shall treat scattering by a general potential.

The idea of using uniform representations was introduced by Langer¹ in 1934, and in a modified form by Cherry² in 1950, to treat problems with one simple turning point. McKelvey³ and Kazarinoff⁴ applied it to a secondorder turning point and to two simple turning points, respectively. All these authors proved that the uniform representation is asymptotic to the exact solution as the wavelength divided by a typical scale length of the potential tends to zero. Their results have been refined and extended by various authors, especially Olver.⁵ The formal aspects of the method have been described by Miller and Good,⁶ and developed futher by Lynn and Keller,⁷ Zauderer,⁸ and Anyanwu and Keller.⁹

In Sec. II we shall write the Schrödinger equation in the form

$$\psi_{xx} + [E - V(x)]\psi = 0.$$
(1)

Here $\psi(x)$ is the wavefunction $E = 2mE'/h^2$, where E' is the particle energy, m is its mass, h is Planck's constant divided by 2π , and $V(x) = 2mV(x)/h^2$, where V'(x) is the potential energy function. In Secs. III and IV we shall set $E = k^2$.

II. BOUND STATES OF A POTENTIAL WELL

Let us begin with the harmonic oscillator, for which we write the potential as $V(x) = x^2/4$ so that Eq. (1) becomes

$$\psi_{xx} + [E - (x^2/4)]\psi = 0. \tag{2}$$

This equation has a solution which vanishes at $x = \pm \infty$ if and only if $E = n + \frac{1}{2}$, where *n* is a non-negative integer. Then ψ is given in terms of the Hermite polynomial He_n(x) by

$$\psi(x) = e^{-(1/4)x^2} \operatorname{He}_n(x). \tag{3}$$

For a general potential well we write the solution $\psi(x)$ of Eq. (1) in the form

$$\psi(x) = \varphi_x^{-1/2} e^{-(1/4)\varphi^2(x)} \operatorname{He}_n[\varphi(x)].$$
(4)

We now substitute Eq. (4) into Eq. (1) and use the fact that expression (3) satisfies Eq. (2) with $E = n + \frac{1}{2}$. Then we find that (4) satisfies Eq. (1) if the new function $\varphi(x)$ satisfies

$$\varphi_x^2[n+\frac{1}{2}-(\varphi^2/4)] = E - V(x) + \varphi_x^{1/2}(\varphi_x^{-1/2})_{xx}.$$
(5)

We now make the assumption that V(x) changes very little in the distance $2\pi E^{-1/2}$, which is the wavelength. This implies that φ_x is also slowly varying on the wavelength scale. Therefore the last term in Eq. (5) is negligible compared to the other two terms, so we omit it and Eq. (5) becomes

$$\varphi_x^2[n+\frac{1}{2}-(\varphi^2/4)] = E - V(x).$$
 (6)

The smallness of the omitted term can be demonstrated by a formal asymptotic analysis in which the wavelength divided by the scale length L of V(x) is introduced as a small parameter. Since we have omitted this small term, Eq. (6) is not actually an equality, but rather it is an asymptotic equality. The difference between the two sides tends to zero as the small parameter $1/E^{1/2}L$ tends to zero. Consequently the same is true of the rest of the equations of Sec. II, since they follow from Eq. (6).

We next suppose that E = V(x) at exactly two points, x_0 and x_1 , with $x_0 < x_1$. These are the classical turning points, and we assume that they are both simple roots. Then the right-hand side of Eq. (6) vanishes at these two points so the left-hand side must also vanish at them. Therefore we shall require that

$$\varphi(x_0) = -2(n+\frac{1}{2})^{1/2}, \quad \varphi(x_1) = 2(n+\frac{1}{2})^{1/2}.$$
 (7)

One of these two conditions may be viewed as an initial condition for $\varphi(x)$, and the other as a condition to determine E.

Now to solve Eq. (6) we take the square root of each side and then integrate from x_0 to x, using Eq. (7) at x_0 . We can integrate the left-hand side explicitly to obtain

$$\frac{1}{4}\varphi\left(n+\frac{1}{2}-\frac{\varphi^2}{4}\right)^{1/2}+\left(n+\frac{1}{2}\right)\sin^{-1}\frac{\varphi}{2(n+1/2)^{1/2}}+\left(n+\frac{1}{2}\right)\frac{\pi}{2}=\int_{x_0}^x [E-V(x)]^{1/2}\,dx.$$
(8a)

Finally we set $x = x_1$ in Eq. (8) and use Eq. (7) at x_1 to get

$$\left(n+\frac{1}{2}\right)\pi = \int_{x_0}^{x_1} [E-V(x)]^{1/2} dx.$$
 (9)

Equation (9) is an equation for the *n*th eigenvalue *E*. Then Eq. (8) determines $\varphi(x)$ and Eq. (4) gives the eigenfunction $\psi(x)$.

In order to solve Eq. (8) explicitly we consider first the case $x > x_1$. Then E < V(x) so the right-hand side of Eq. (8) is imaginary and large in magnitude. We can satisfy Eq. (8) if φ is large and positive, for then the left-hand side is ap-

proximately $i\varphi^2/8$, and Eq. (8) yields

$$\varphi^{2}(x) \approx 8 \int_{x_{1}}^{x} [V(x) - E]^{1/2} dx.$$
 (8b)

When this result is used in Eq. (4) it gives an exponentially small value for $\psi(x)$.

For $x \ll x_0$ we find instead that φ is large and negative, and that Eq. (8b) holds with the integration from x to x_0 . Then Eq. (4) again yields an exponentially small result for $\psi(x)$. When x lies between x_0 and x_1 , $\varphi(x)$ is between the values given in Eq. (7). It can be found by solving Eq. (8a) numerically.

III. SCATTERING BY A PARABOLIC POTENTIAL BARRIER

We now consider the parabolic potential barrier, which we write as $V(x) = k^2 + a - x^2/4$. We denote $\psi(x)$ by E(a,x); then Eq. (1) becomes

$$E_{xx}(a,x) + [(x^2/4) - a]E(a,x) = 0.$$
(10)

The constant a equals the maximum value of the potential minus the particle energy k^2 .

Equation (10), like Eq. (2), is called the parabolic cylinder or Weber equation and its solutions are called parabolic cylinder or Weber functions. These functions have been studied extensively and tabulated, e.g., in Abramowitz and Stegun, ¹⁰ Chap. 19. One of the standard solutions, E(a,x), behaves like an oscillatory exponential function with increasing phase for x large and positive. Thus it represents a wave traveling to the right in this range, so we may think of it as the transmitted wave. To determine its behavior for negative values of x, we use Eq. (19.18.3) of Ref. 10:

$$(1+e^{2\pi a})^{1/2}E(a,x)=e^{\pi a}E^{*}(a,x)+iE^{*}(a,-x).$$
 (11)

We take the complex conjugate of Eq. (11) and then solve for E(a, -x) to get

$$E(a, -x) = i(1 + e^{2\pi a})^{1/2} E^{*}(a, x) - i e^{\pi a} E(a, x). \quad (12)$$

For x > 0, Eq. (12) determines E for the negative argument -x as the sum of two waves. We shall see in a moment that in Eq. (12) $E^{*}(a,x)$ represents a wave traveling to the right and E(a,x) represents a wave traveling to the left, so we can call them the incident and reflected waves, respectively. The absolute value of the ratio of these two waves is |R|, where R is the complex reflection coefficient. Thus we have from Eq. (12),

$$|\mathbf{R}| = e^{\pi a} / (1 + e^{2\pi a})^{1/2}.$$
 (13)

Similarly, the absolute value of the transmitted wave E(a,x) divided by the incident wave is |T|, where T is the complex transmission coefficient. We see from Eq. (12) that

$$|T| = 1/(1 + e^{2\pi a})^{1/2}.$$
 (14)

These two results show that $|R|^2 + |T|^2 = 1$, which expresses conservation of probability.

To examine the solution in more detail, we write it in the following form for $x \ge |a|$ [Ref. 10, Eq. (19.21.1)]:

$$E(a,x) = \exp\left[i\left(\frac{\phi}{2} + \frac{\pi}{4}\right)\right] \cdot s(a,x)\left(\frac{2}{x}\right)^{1/2}$$
$$\times \exp\left[i\left(\frac{x^2}{4} - a\ln x\right)\right], \quad x \ge |a|. \tag{15}$$

Here ϕ is a real constant defined in terms of the gamma

function by

$$\phi = \arg \Gamma(1/2 + ia), \quad \phi = 0 \text{ for } a = 0.$$
The function $s(a,x)$ tends to unity as $x \to +\infty$:
(16)

 $s(a,x) = 1 + O(1/x^2), \quad x \to +\infty.$

By using Eq.
$$(15)$$
 in Eq. (12) we get

$$E(a, -x) = i(1 + e^{2\pi a})^{1/2} \exp\left[-i\left(\frac{\phi}{2} + \frac{\pi}{4}\right)\right] s^{\bullet}(a, x) \left(\frac{2}{x}\right)^{1/2} \exp\left[-i\left(\frac{x^2}{4} - a\ln x\right)\right] - ie^{\pi a} \exp\left[i\left(\frac{\phi}{2} + \frac{\pi}{4}\right)\right] s(a, x) \left(\frac{2}{x}\right)^{1/2} \exp\left[i\left(\frac{x^2}{4} - a\ln x\right)\right], \quad -x < -|a|.$$
(18)

Equation (15) shows that the phase of E increases with x for x > |a|, so E does represent a wave traveling to the right there. Similarly the first term in Eq. (18) has a phase which increases as -x increases so it is also a rightward traveling wave, as we stated above. The second term is a leftward traveling wave. However, the phases do not become linear in x for large x, and therefore the waves do not tend to free waves. This is to be expected because the parabolic potential does not decay, but instead grows at infinity. Therefore we cannot define complex R and T in the usual way, but we can define |R| and |T|, as we have shown above.

IV. SCATTERING BY A GENERAL POTENTIAL

For a general potential we write the solution $\psi(x)$ of Eq. (1) in terms of E(a,x) in the form

$$\psi(x) = \varphi_x^{-1/2} E[a, \varphi(x)].$$
(19)

Here $\varphi(x)$ is a function to be determined so that $\psi(x)$ satisfies Eq. (1). Substitution of Eq. (19) into Eq. (1), and the use of Eq. (10), shows that ψ is a solution if $\varphi(x)$ satisfies

$$\varphi_x^2[(\varphi^2/4) - a] = k^2 - V(x) + \varphi_x^{1/2}(\varphi_x^{-1/2})_{xx}.$$
(20)

When V(x) is slowly varying, and therefore $\varphi_x(x)$ is also, we neglect the last term in Eq. (20) and obtain

$$\varphi_x^2[(\varphi^2/4) - a] = k^2 - V(x).$$
(21)

As was the case with Eq. (6) in Sec. II, Eq. (21) is not an equality but instead the two sides become asymptotically equal as 1/kL tends to zero. Here L is a typical scale length of the potential V(x) and k is 2π divided by the incident wavelength λ . Thus Eq. (2) is more correct the smaller the

ratio $\lambda / 2\pi L$. The same is true of all the subsequent equations of Sec. IV, since they all depend upon Eq. (21).

(17)

We now assume that for $k^2 < \max V(x)$, there are two simple roots x_0 and x_1 of $k^2 = V(x)$, with $x_0 < x_1$. At these turning points the right-hand side of Eq. (21) vanishes, so to make the left side vanish there we require that a > 0 and that

$$\varphi(x_0) = -2a^{1/2}, \quad \varphi(x_1) = 2a^{1/2}.$$
 (22)

When $k^2 = \max V(x)$ then $x_0 = x_1$ is a double root or second-order turning point, and Eq. (22) still applies with a = 0.

When $k^2 > \max V(x)$, we assume that V(x) is analytic in some strip containing the real axis, and that $V(x) = k^2$ has a pair of complex conjugate roots in this strip. If there are more than one pair we choose that pair closest to the real axis and call them x_0 and x_1 with Im $x_0 < 0$. Then we require a < 0 and we still impose Eq. (22).

We now solve Eq. (21) for $a > \bar{0}$ by taking the square roots of both sides and then integrating from x_1 to $x > x_1$. Upon using Eq. (22) we obtain

$$\int_{x_1}^{x} [k^2 - V(x)]^{1/2} dx$$

= $\frac{1}{4} \varphi(\varphi^2 - 4a)^{1/2} - a \ln \frac{\varphi + (\varphi^2 - 4a)^{1/2}}{2a^{1/2}}, \ x > x_1,$
 $\sim \frac{\varphi^2}{4} - a \ln \varphi + \frac{a}{2} (\ln a - 1), \ x > x_1.$ (23)

The second form of Eq. (23) follows from the first because $\varphi > a^{1/2}$ when $x > x_1$. To find φ for $x < x_0$ we again take the square roots of both sides of Eq. (21) and integrate from x to x_0 to get

$$\int_{x}^{x_{0}} [k^{2} - V(x)]^{1/2} dx = -\frac{1}{4} \varphi(\varphi^{2} - 4a)^{1/2} - a \ln \frac{-\varphi + (\varphi^{2} - 4a)^{1/2}}{2a^{1/2}}, \quad x < x_{0},$$
$$\sim \frac{\varphi^{2}}{4} - a \ln(-\varphi) + \frac{a}{2} (\ln a - 1), \quad x < x_{0}.$$
(24)

For x between x_0 and x_1 we obtain

$$\int_{x_0}^x [V(x) - k^2]^{1/2} dx = \frac{\varphi}{4} (4a - \varphi^2)^{1/2} + a \sin^{-1} \frac{\varphi}{2a^{1/2}} + \frac{\pi a}{2}, \quad x_0 \le x \le x_1.$$
(25)

It should be noted that Eqs. (23)–(25) for $\varphi(x)$ are just different forms of one single equation which has been written in different ways for convenience.

By setting $x = x_1$ in Eq. (25) and using Eq. (22) we get an expression for a:

$$\pi a = \int_{x_0}^{x_1} [V(x) - k^2]^{1/2} dx.$$
(26)

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This completes the determination of the solution $\psi(x)$. It is given by Eq. (19) with $\varphi(x)$ given by Eqs. (23), (24), or (25) and with a given by Eq. (26). It was derived for $k^2 < \max V(x)$, in which case a > 0, but it also holds for $k^2 = \max V(x)$ when a = 0. The changes needed when $k^2 > \max V(x)$ are derived in the Appendix.

The asymptotic form of $\psi(x)$ for $x \ge x_1$ is obtained by using Eq. (15) for E with φ determined by the second form of Eq. (23). This yields

$$\psi(x) \sim \left(\frac{2}{\varphi \varphi_x}\right)^{1/2} \exp\left[i \left(\int_{x_1}^x [k^2 - V(x)]^{1/2} dx + \frac{\phi}{2} + \frac{\pi}{4} - \frac{a}{2} \ln \frac{a}{e}\right)\right], \quad x > x_1.$$
(27)

To calculate $\varphi \varphi_x/2$ we differentiate the second form of Eq. (23), neglecting a/φ , and we obtain $\varphi \varphi_x/2 \sim k$ provided that V(x) tends to zero as $x \to \infty$. Then we add and subtract k to the integrand in Eq. (27), and we can write the result in the form

$$\psi(x) \sim k^{-1} \exp\left[i \left(\int_{x_1}^{\infty} \{ [k^2 - V(x)]^{1/2} - k \} dx + k(x - x_1) + \frac{\phi}{2} + \frac{\pi}{4} - \frac{a}{2} \ln \frac{a}{e}, \quad x > x_1. \right]$$
(28)

The upper limit in the integral has been changed from x to ∞ , which is permissible if V(x) tends to zero fast enough for the integral to converge. In the same way, we use Eq. (18) for E and Eq. (24) for φ to obtain

$$\psi(x) \sim ik^{-1}(1+e^{2\pi a})^{1/2} \exp\left\{i\left[-\int_{-\infty}^{x_0} \left\{\left[k^2-V(x)\right]^{1/2}-k\right\}dx+k(x-x_0)-\left(\frac{\phi}{2}+\frac{\pi}{4}\right)+\frac{a}{2}\ln\frac{a}{e}\right]\right\}$$
$$-ik^{-1}e^{\pi a} \exp\left[i\left(\int_{-\infty}^{x_0} \left\{\left[k^2-V(x)\right]^{1/2}-k\right\}dx-k(x-x_0)+\frac{\phi}{2}+\frac{\pi}{4}-\frac{a}{2}\ln\frac{a}{e}\right)\right], \quad x \ll x_0.$$
(29)

The reflection coefficient R is the ratio of the coefficient of e^{-ikx} to that of e^{ikx} in Eq. (29), which is

$$R = \frac{-i \exp[\pi a + i\phi - ia \ln(a/e)]}{(1 + e^{2\pi a})^{1/2}} \times \exp 2i \left(\int_{-\infty}^{x_0} \{ [k^2 - V(x)]^{1/2} - k \} dx + kx_0 \right).$$
(30)

Similarly T is the ratio of the coefficient of e^{ikx} in Eq. (28) to that of e^{ikx} in Eq. (29):

$$T = \frac{\exp[i\phi - ia \ln(a/e)]}{(1 + e^{2\pi a})^{1/2}}$$

 $\times \exp i \left(\int_{-\infty}^{x_0} \{ [k^2 - V(x)]^{1/2} - k \} dx - k(x_1 - x_0) + \int_{x_1}^{\infty} \{ [k^2 - V(x)]^{1/2} - k \} dx \right).$
(31)

From these results we see that Eqs. (13) and (14) still hold with πa given Eq. (26), and that $|R|^2 + |T|^2 = 1$.

The phase of T can be written in the following form, using Eq. (16) for ϕ :

$$\arg T = \int_{-\infty}^{\infty} \{\operatorname{Re}[k^{2} - V(x)]^{1/2} - k\} dx + \arg \Gamma\left(\frac{1}{2} + ia\right) - a \ln\left(\frac{a}{e}\right).$$
(32)

The phase of R is

$$\arg R = 2 \int_{-\infty}^{x_0} \{ [k^2 - V(x)]^{1/2} - k \} dx + 2kx_0 + \arg \Gamma \left(\frac{1}{2} + ia \right) - \frac{\pi}{2} - a \ln \left(\frac{a}{e} \right).$$
(33)

We note that $\arg \Gamma(\frac{1}{2} + ia) = 0$ for a = 0 and $\arg \Gamma(\frac{1}{2} + ia) \sim a \log(a/e)$ for a real and |a| > 1. The term $2kx_0$ in Eq. (33) shows that $\arg R$ depends upon the location of the origin of x, so it is not a property of the potential alone. However, $\arg T$ depends only upon V(x) and k.

When $k^2 > \max V(x)$, Eqs. (30)–(33) still hold with x_0 and x_1 both replaced by Re x_0 , and with a given by

$$\pi a = -\int_{-\operatorname{Im} x_0}^{\operatorname{Im} x_0} [k^2 - V(\operatorname{Re} x_0 + is)]^{1/2} \, ds. \qquad (34)$$

The integral is real and positive, so *a* is real and negative. In Eq. (32) the sign Re can be omitted since $k^2 > V(x)$ for all real *x*. These are shown in the Appendix.

V. CONCLUSION

We have now shown how to solve the one-dimensional Schrödinger equation for potentials which change little within a distance of one wavelength. This is exactly the case for which the WKB method was devised. However, that method requires the use of many different representations of the solution in different regions of space, with connection formulas to match them together. In each of the present examples it would require five such representations. By contrast, the uniform method we have presented requires only one representation.

In the bound state problem the result (9) for the eigenvalues is the same as that given by the WKB method. But the present derivation is simpler. Furthermore, the representation (4) for the wavefunction is valid for all x.

In the scattering problem the results (30) and (31) for Rand T hold for all incident particle energies k^2 . These results also contain the phases of R and T, which do not seem to be given elsewhere. In addition the representation (19) for $\psi(x)$ holds for all x.

Suppose we wanted to find the bound states of a double well, or to treat scattering by a double barrier. In both cases there would be four turning points, and the WKB method

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would require nine representations of the solution. By using the present method, it would be possible to use just one representation if one had available special functions with four turning points. However, such functions have hardly been studied, so that is not feasible. Instead one could use two representations, each covering a region containing two turning points, so parabolic cylinder functions would suffice. Of course, they would have to be matched together. This procedure could be extended to more complicated potentials.

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APPENDIX

When $k^2 > \max V(x)$ and a < 0 all three forms (23)– (25) of the integral of (21) hold for all x in the region of analyticity of V(x). The asymptotic forms hold for $|\operatorname{Re} x| > |\operatorname{Re} x_0|$. Upon setting $x = \operatorname{Re} x_0 + is$ in (26) we obtain

$$\pi a = -\int_{-\operatorname{Im} x_0}^{\operatorname{Im} x_0} [k^2 - V(\operatorname{Re} x_0 + is)]^{1/2} \, ds. \qquad (A1)$$

Because V(z) is analytic and real for real z, its power series about any real point has all real coefficients. It follows from this that $V^*(x + iy) = V(x - iy)$, which implies that the real part of V is even in y and the imaginary part is odd. Then we find that the imaginary part of the integral in Eq. (A1) is zero because the range of integration is symmetric about the real axis.

To solve Eq. (21) for $\varphi(x)$ we just integrate from the point Re x_0 on the real axis, and we obtain

$$\int_{\operatorname{Re} x_{0}}^{x} [k^{2} - V(x)]^{1/2} dx$$

= $\frac{1}{4} \varphi(\varphi^{2} - 4a)^{1/2} - a \ln[\varphi + (\varphi^{2} - 4a)^{1/2}] - \Phi$
 $\sim \frac{\varphi^{2}}{4} - a \ln \varphi + \frac{a}{2} \ln \frac{a}{e} - \Phi, \quad |\varphi| \ge |a|.$ (A2)

Here Φ is defined in terms of $\varphi_0 = \varphi(\operatorname{Re} x_0)$ by

$$\Phi = \frac{1}{4}\varphi_0(\varphi_0^2 - 4a)^{1/2} - a\ln[\varphi_0 + (\varphi_0^2 - 4a)^{1/2}].$$
(A3)

The value of φ_0 can be found by integrating Eq. (21) from x_0 , where φ is known, to Re x_0 .

When the second form of Eq. (A2) is used in (19) for x large and positive, it yields Eq. (27) with x_1 replaced by Re x_0 and with the additional phase Φ . Then Eq. (28) follows with these same changes. When the second form of Eq. (A2) is used in (19) for x large and negative, Eq. (29) results with x_0 replaced by Re x_0 and with the extra phase Φ in each term. This phase cancels out of R and T, which are still given by Eqs. (30) and (31) with x_0 and x_1 both replaced by Re x_0 .

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A simple formula for combining rotations and Lorentz boosts

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We present a simple formula which is helpful in understanding the result of combining two Lorentz transformations, in particular two rotations or two Lorentz boosts. In the latter case the Wigner little group rotation occurs naturally. The formulas for the resultant angle of rotation and rapidity are generalizations of trigonometric addition theorems and of the relativistic law for adding collinear velocities.

In their book on gravitation, Misner *et al.*¹ recall how pondering on the problem of finding the correct law for combining rotations led Hamilton to the invention of quaternions in 1843. They describe the problem as follows. Consider a rotation of 90° about the *z* axis, followed by one of 90° about the *x* axis. To what single rotation does this operation correspond? If rotations combined like vectors the resultant axis of rotation would lie in the x-z plane and the angle of rotation would be $\sqrt{2} \times 90^{\circ} = 127.28^{\circ}$. Actually the axis of rotation is in the (1, -1, 1) direction and the angle of rotation is 120°. "What computational algorithm," ask the authors, "can ever reproduce a law of combination of rotations apparently so strange?"

Up to the present day Hamilton's quaternion calculus,