Inaccurate use of asymptotic formulas

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(Received 15 December 2003; accepted 2 February 2004)

The asymptotic form of the plane wave decomposition into spherical waves, which is used to express the scattering amplitude in terms of phase shifts, is incorrect. We explain why and show how to circumvent the mathematical inconsistency.
[DOI: 10.1119/1.1688785]

In quantum mechanics the following plane wave decomposition into spherical waves is used

$$e^{i\mathbf{k}\cdot\mathbf{r}}=\sum_{l=0}^{\infty} i^l(2l+1)P_l(\cos\Theta)j_l(kr), \tag{1}$$

where $\mathbf{k}\cdot\mathbf{r}=kr\cos\Theta$, P_l is the lth Legendre polynomial, and j_l is the lth spherical Bessel function. Because we are interested in the large distance behavior of the wave function in scattering theory, we need the asymptotic form of the spherical function

$$j_l(kr)\approx\frac{\sin(kr-\pi l/2)}{kr}, \tag{2}$$

and we rewrite Eq. (1) as

$$e^{i\mathbf{k}\cdot\mathbf{r}}\overset{?}{\approx}\frac{1}{kr}\sum_{l=0}^{\infty} i^l(2l+1)P_l(\cos\Theta)\sin(kr-\pi l/2). \tag{3}$$

Equation (3) is given in numerous textbooks on quantum mechanics, including those of Schiff[1] and Landau and Lifshitz.[2] Astonishingly, expression (3) is meaningless, and for this reason we put the question mark over the approximate equality. The series is not only divergent, but it cannot even be treated as an asymptotic expansion of the function $e^{i\mathbf{k}\cdot\mathbf{r}}$ at large distances.

To see how badly the series (3) diverges, we consider the special case $\cos\Theta=1$. Then, $P_l(1)=1$, and after a simple calculation we obtain

$$e^{ikr}\overset{?}{\approx}\frac{\sin(kr)}{kr}\sum_{l=0}^{\infty}(2l+1)\cos^2(\pi l/2) -i\,\frac{\cos(kr)}{kr}\sum_{l=0}^{\infty}(2l+1)\sin^2(\pi l/2) \tag{4a}$$

$$=\frac{\sin(kr)}{kr}\sum_{n=0}^{\infty}(4n+1)-i\,\frac{\cos(kr)}{kr}\sum_{n=0}^{\infty}(4n+3). \tag{4b}$$

According to Eq. (4), both the real and imaginary parts of e^{ikr} contain a divergent series, for any value of r.

However, we often consider asymptotic series that are divergent, but still correctly represent certain functions. The infinite series $a_0(x)+a_1(x)+a_2(x)+\cdots$ is the asymptotic expansion of the function $f(x)$ at x_0 (which can be infinite) if[3]

$$\frac{1}{a_n(x)}\left(f(x)-\sum_{l=0}^{n} a_l(x)\right)\to 0 \quad \text{for } x\to x_0. \tag{5}$$

Equivalently, the series is asymptotic if

$$\frac{a_{l+1}(x)}{a_l(x)}\to 0 \quad \text{for } x\to x_0. \tag{6}$$

Due to the definition (5), any finite subseries of an asymptotic series approximates the function $f(x)$ and the approximation becomes better and better as $x\to x_0$. However, the series (3) does not satisfy the condition (6), and consequently, it cannot be treated as an asymptotic expansion of $e^{i\mathbf{k}\cdot\mathbf{r}}$ at large distances.

What is wrong with the expansion (3)? It appears that the approximate formula (2) requires that

$$kr\gg\tfrac{1}{2}l(l+1). \tag{7}$$

For completeness, we derive this condition here, and find not only the first but also the second term of the $1/z$ expansion of $j_l(z)$. It is well known (see, for example, Ref. 4) that the spherical Bessel functions can be written as

$$j_l(z)=z^l\left(-\frac{1}{z}\frac{d}{dz}\right)^l\frac{\sin z}{z}. \tag{8}$$

If we use Eq. (8) and the recursion formula,

$$j_{l+1}(z)=-z^l\frac{d}{dz}\left(\frac{1}{z^l}j_l(z)\right), \tag{9}$$

we can easily prove by induction that

$$j_l(z)=\frac{\sin(z-\pi l/2)}{z}+\frac{1}{2}l(l+1)\frac{\cos(z-\pi l/2)}{z^2}+\mathcal{O}\left(\frac{1}{z^3}\right). \tag{10}$$

If we compare the two terms of the expansion (10), we find that the approximation (2) holds if the condition (7) is satisfied. When we perform the summation in Eq. (3), we find that the terms for sufficiently large l violate the requirement (7), and effectively destroy even the approximate equality.

Although the decomposition (3) is incorrect, the results obtained by means of it are usually correct. Obviously, the famous formula that expresses the scattering amplitude via the phase shifts is correct. However, it is of interest to see why the derivation works. Therefore, we first discuss the standard procedure, which can be found, for example, in Refs. 1 and 2, and then we show how to avoid the mathematical inconsistency.

By assuming azimuthal symmetry, the scattered wave function is

$$\phi_{\mathbf{k}}(\mathbf{r}) = \sum_{l=0}^{\infty} A_l i^l (2l+1) P_l(\cos\Theta) R_l(r), \tag{11}$$

where the R_l are the radial wave functions and the A_l are coefficients to be determined. If we assume that the asymptotics of the radial functions are

$$R_l(r) \approx \frac{\sin(kr - \pi l/2 + \delta_l)}{kr}, \tag{12}$$

where δ_l denotes the lth phase-shift, we can rewrite Eq. (11) as

$$\phi_{\mathbf{k}}(\mathbf{r}) \overset{?}{\approx} \frac{1}{kr} \sum_{l=0}^{\infty} A_l i^l (2l+1) P_l(\cos\Theta) \times \sin(kr - \pi l/2 + \delta_l). \tag{13}$$

We still put the question mark over the equalities that are mathematically inappropriate.

Now, we compare the wave function (13) with the expected asymptotic form of the scattered wave function

$$\phi_{\mathbf{k}}(\mathbf{r}) = e^{i\mathbf{kr}} + f(\Theta) \frac{e^{ikr}}{r}, \tag{14}$$

where $f(\Theta)$ is the scattering amplitude. If we use the plane-wave decomposition (3), we find

$$\frac{1}{kr} \sum_{l=0}^{\infty} A_l i^l (2l+1) P_l(\cos\Theta) \sin(kr - \pi l/2 + \delta_l) \overset{?}{\approx} \frac{1}{kr} \sum_{l=0}^{\infty} i^l (2l+1) P_l(\cos\Theta) \sin(kr - \pi l/2) + f(\Theta) \frac{e^{ikr}}{r}. \tag{15}$$

If we equate the terms proportional to e^{-ikr}, we find that $A_l = e^{i\delta_l}$, which when substituted into the terms proportional to e^{ikr}, provides the well-known result

$$f(\Theta) = \frac{1}{2ik} \sum_{l=0}^{\infty} (2l+1) P_l(\cos\Theta) [e^{2i\delta_l} - 1]. \tag{16}$$

We obtained relation (16) using the mathematically meaningless equations (3), (13), and (15). Next, we show how to derive Eq. (16) avoiding the inconsistency.

Again we start with the wave function in the form (11), and we use the asymptotics of the radial wave function (12), but only for fixed values of l. For this reason we calculate the projection

$$\int_{-1}^{+1} d(\cos\Theta)\, \phi_{\mathbf{k}}(\mathbf{r}) P_l(\cos\Theta) = 2 i^l A_l R_l(r), \tag{17}$$

where we have taken into account that the Legendre polynomials are orthogonal

$$\int_{-1}^{+1} d(\cos\Theta) P_l(\cos\Theta) P_{l'}(\cos\Theta) = \frac{2}{2l+1} \delta^{ll'}. \tag{18}$$

We decompose the scattering amplitude,

$$f(\Theta) = \frac{1}{2ik} \sum_{l=0}^{\infty} C_l i^l (2l+1) P_l(\cos\Theta), \tag{19}$$

and we project the scattered wave function (14) as

$$\int_{-1}^{+1} d(\cos\Theta) \left(e^{i\mathbf{kr}} + f(\Theta) \frac{e^{ikr}}{r} \right) P_l(\cos\Theta) = 2 i^l \left(j_l(kr) + C_l \frac{e^{ikr}}{r} \right). \tag{20}$$

Next, we equate the asymptotic forms of the projections (17) and (20), and thus, instead of Eq. (15), we obtain

$$A_l \sin(kr - \pi l/2 + \delta_l) = \sin(kr - \pi l/2) + C_l k \frac{e^{ikr}}{r}. \tag{21}$$

We compare the terms proportional to e^{-ikr} and e^{ikr}, respectively, and find that $A_l = e^{i\delta_l}$ and

$$C_l = \frac{1}{2ik} e^{-i\pi l/2} [e^{2i\delta_l} - 1], \tag{22}$$

which, due to Eq. (19), again provides the correct result (16).

Although the problem discussed here looks purely academic it was discovered in the course of concrete calculations. To simplify the calculation of a correlation function where the scattering wave function enters, we used the form (13) with $A_l = e^{i\delta_l}$ as is given in many books. We were interested in the complete sum of partial waves, and we used Eq. (13) instead of Eq. (14) to exploit the orthogonality of Legendre polynomials. Needless to say the calculation went wrong, showing that the asymptotic expressions must be treated very carefully.

ACKNOWLEDGMENTS

We are very grateful to Konrad Bajer and Iwo Białynicki-Birula for correspondence and stimulating criticism.

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