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GENERALIZED AIRY FUNCTIONS FOR USE IN ONE-DIMENSIONAL QUANTUM MECHANICAL PROBLEMS *

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ABSTRACT

The solution of the one-dimensional time-independent Schrödinger equation in which the energy minus the potential varies as the n-th power of the distance is obtained from proper linear combinations of Bessel functions of order $(n + 2)^{-1}$. The linear combinations, which we call "generalized Airy functions" $\mathcal{A}i_\nu(x)$ and $\mathcal{B}i_\nu(x)$, reduce to the usual Airy functions $Ai(x)$ and $Bi(x)$ when $n = 1$ and have the same type of simple asymptotic behavior. Expressions for the generalized Airy functions which can be evaluated by the method of generalized Gaussian quadrature are obtained.

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I

GENERALIZED AIRY FUNCTIONS FOR USE IN ONE-DIMENSIONAL QUANTUM MECHANICAL PROBLEMS

For one-dimensional quantum mechanical systems, the usual WKB approximation gives simple expressions for the wave function in both the classical and the non-classical regions of configuration space. Connection formulas relate the two expressions on either side of a classical turning point where the WKB wavefunctions become infinite. The standard textbook[1] example of the connection formulas in the semi-classical approach assumes that the potential is a linear function of x in the neighborhood of the turning point. The exact solution in this case is given by the Airy functions $Ai(x)$ and $Bi(x)$ which are simply related to Bessel functions of order 1/3. An analogous treatment for the Schrödinger equation

$$\frac{d^2w(x)}{dx^2} + c^2x^n \ w(x) = 0 \quad , \qquad (1)$$

where $c^2x^n \equiv Q^2(x) = \frac{2\mu}{\hbar^2}[E - V(x)]$ has a zero of order n is easily obtained but does not seem to be readily available. In this note explicit expressions for the solution of Eq. (1) for which Q^2 has a zero of arbitrary order are obtained. We call these solutions "generalized Airy functions" $\mathcal{A}i_\nu(x)$ and $\mathcal{B}i_\nu(x)$ since they are standardized to give the Airy functions for $n = 1$. Gordon[2] has given a method for calculating the Airy functions by means of generalized Gaussian quadrature. This method is extended here for the calculation of the generalized Airy functions.

In the following development it is shown that the generalized Airy functions are linear combinations of solutions $w_\nu \pm (x)$ to Eq. (1),

$$\begin{aligned} \mathcal{A}i_\nu(x) &= k_1\,[w_\nu^{+}(x) + w_\nu^{-}(x)] \\ \mathcal{B}i_\nu(x) &= k_2\,[w_\nu^{-}(x) - w_\nu^{+}(x)] \end{aligned} \qquad , \tag{2}$$

where the k's are constants and the $w_\nu^{\pm}$ are proportional to real solutions $u_\nu^{\pm}(x)$ (valid in the classical region) and $v_\nu^{\pm}(x)$ (valid in the non-classical region). The constants of proportionality are determined so that the $w_\nu^{\pm}$ remain well-behaved in passing through the turning point, $x = 0$.

For convenience we take the non-classical region to be to the left of the origin. The solution of Eq. (1) with c real was found by Lommel[3] to be:

$$w_\nu^{\pm}(x > 0) \equiv A_{\pm}\, u_\nu^{\pm} = A_{\pm}\,(\xi/Q)^{1/2}\, J_{\pm}\,(\xi) \tag{3}$$

where $\xi = \int_0^x Q(x)\,dx$, $\nu^{-1} = n + 2$, $A_{\pm}$ are constants, and the $J_{\pm\nu}$ are Bessel functions of real argument. In the non-classical region this solution takes the real form

$$w_\nu^{\pm}(x < 0) \equiv B_{\pm} v_\nu^{\pm}(x) = B_{\pm}(|\xi|/|Q|)^{1/2}\, I_{\pm\nu}(|\xi|) \tag{4}$$

where $|\xi| = \int_x^0 |Q(x)|dx$, $B_{\pm}$ are constants, and $I_{\pm\nu}(z) = \exp(-\pi\nu i/2)\, J_{\pm\nu}(iz)$ are Bessel functions of imaginary argument.

Watson[4] gives the following limiting forms of these Bessel functions:

$x \to 0$

$$J_{\pm\nu}(\xi) = \frac{(\frac{1}{2}\,\xi)^{\pm\nu}}{\Gamma(1 \pm \nu)} + \dots$$
$$I_{\pm\nu}(|\xi|) = \frac{(\frac{1}{2}\,|\xi|)^{\pm\nu}}{\Gamma(1 \pm \nu)} + \dots \tag{5}$$

$x \to \infty$

$$J_{\pm\nu}(\xi) = (\frac{2}{\pi\xi})^{1/2} \cos(\xi \mp \nu\pi/2 - \pi/4) + \dots \tag{6}$$

$x \to -\infty$

$$I_{\pm\nu}(|\xi|) = (2\pi|\xi|)^{-1/2} \{ e^{|\xi|}[1+0(\frac{1}{|\xi|})] + e^{[-|\xi|-(\frac{1}{2} \pm \nu)\pi i]} + \dots\} . \tag{7}$$

A derivation of the connection formulas, originally due to Jeffreys,[5] uses the limiting forms near the turning point. Expanding the $w_\nu^{\pm}(x)$ of Eqs. (3) and (4) in powers of x , we obtain as leading terms

$$w_\nu^{+}(x > 0) = A_+ \, (2\nu)^{1/2} \, (c\nu)^{\nu} \, x/\Gamma(1 + \nu) + \dots$$
$$w_\nu^{-}(x > 0) = A_- \, (2\nu)^{1/2} \, (c\nu)^{-\nu}/\Gamma(1 - \nu) + \dots$$
$$w_\nu^{+}(x < 0) = B_+ \, (2\nu)^{1/2} \, (c\nu)^{\nu} \, |x|/\Gamma(1 + \nu) + \dots \tag{8}$$
$$w_\nu^{-}(x < 0) = B_-(2\nu)^{1/2} \, (c\nu)^{\nu}/\Gamma(1 - \nu) + \dots .$$

A connection formula arises from the condition that these different solutions join smoothly at the turning point. This condition is satisfied for $w_\nu^+(x > 0)$ and $w_\nu^+(x < 0)$ if $B_+ = - A_+$ and for $w_\nu^-(x > 0)$ and $w_\nu^-(x < 0)$ if $A_- = B_-$. It is convenient to take the magnitudes of these constants as unity. Now the explicit expressions for the $w_\nu^\pm$ in terms of the Bessel functions are

$$
\begin{aligned}
w_\nu^+(x > 0) &= u_\nu^+(x) = (\xi/Q)^{1/2} J_{+\nu}(\xi) \\
w_\nu^-(x > 0) &= u_\nu^-(x) = (\xi/Q)^{1/2} J_{-\nu}(\xi)
\end{aligned}
\qquad (3')
$$

$$
\begin{aligned}
w_\nu^+(x < 0) &= -v_\nu^+(x) = - (|\xi|/|Q|)^{1/2} I_{+\nu}(|\xi|) \\
w_\nu^-(x < 0) &= v_\nu^-(x) = (|\xi|/|Q|)^{1/2} I_{-\nu}(|\xi|)
\end{aligned}
\qquad (4')
$$

The asymptotic behavior of the $w_\nu^\pm$ functions follows from Eqs. (6) and (7):

$x \to \infty$

$$
\begin{aligned}
w_\nu^+ &= (\tfrac{1}{2}\pi Q)^{-1/2} \cos(\xi - \nu\pi/2 - \pi/4) + \ldots \\
w_\nu^- &= (\tfrac{1}{2}\pi Q)^{-1/2} \cos(\xi + \nu\pi/2 - \pi/4) + \ldots
\end{aligned}
\qquad (9)
$$

$x \to -\infty$

$$
\begin{aligned}
w_\nu^+ &= -(2\pi|Q|)^{-1/2} \{ e^{|\xi|}[1 + O(\tfrac{1}{|\xi|})] + \{ e^{[-|\xi|-(\frac{1}{2} + \nu)\pi i]} + \ldots\} \\
w_\nu^- &= (2\pi|Q|)^{-1/2} \{ e^{|\xi|}[1 + O(\tfrac{1}{|\xi|})] + \{ e^{[-|\xi|-(\frac{1}{2} - \nu)\pi i]} + \ldots\} .
\end{aligned}
\qquad (10)
$$

We now wish to find linear combinations of these functions which are suitable for describing wave functions. If there is no turning point to the left of the origin, one combination must yield a decaying exponential in the non-classical region. The linear combination $w_\nu^+ + w_\nu^-$ has the asymptotic behavior

$x \to -\infty$

$$w_\nu^+ + w_\nu^- = 2\sin(\nu\pi)\ (2\pi|Q|)^{-1/2}\quad e^{-|\xi|} + \ldots \tag{11}$$

$x \to \infty$

$$w_\nu^+ + w_\nu^- = 2\cos(\nu\pi/2)\ (\tfrac{1}{2}\pi Q)^{-1/2}\cos(\xi - \pi/4) + \ldots \tag{12}$$

As usually stated, the connection formula in this case would have the form:

$$\sin(\nu\pi/2)\ |Q|^{-1/2}\quad e^{-|\xi|} \to Q^{-1/2}\cos(\xi - \pi/4)\quad . \tag{13}$$

The one-sided nature of this connection formula is meant to imply the following: if the expression on the left is a good asymptotic approximation to the true solution to the left of the turning point, then the expression on the right is a good asymptotic approximation to the right of the turning point. However, it is not possible to apply the converse, that is, to reverse the arrow. The reason for this bias in direction is not clear from Jeffreys' derivation (Jeffreys used a double-head arrow), but is explained in Langer's article[6] where the case for $\nu = 1/3$ is treated. It is sufficient to state here that when the arrow is reversed in Eq. (13) the increasing exponential term in $w_\nu^{\pm}$ is introduced if the phase of the wave function is only slightly different from $\pi/4$. The connection formula problem is interesting from a mathematical viewpoint but is unimportant in practice.

In obvious analogy to the usual Airy functions we identify the $\mathcal{A}i_\nu$ as the linear combination $w_\nu^{+} + w_\nu^{-}$ and the $\mathcal{B}i_\nu$ as the linear combination $w_\nu^{-} - w_\nu^{+}$. Choosing $k_1 = 2^{-3/2}\csc(\nu\pi)$ and $k_2 = 2^{-1/2}$ as the constants in Eq. (2), the following expressions are obtained:

$$\mathcal{A}i_\nu(-x) = \frac{1}{2}\csc(\nu\pi)\ \nu^{1/2}\ x^{1/2}[I_{-\nu}(\xi) - I_\nu(\xi)]$$

$$\mathcal{A}i_\nu(x) = \frac{1}{2}\csc(\nu\pi)\ \nu^{1/2}\ x^{1/2}[J_\nu(\xi) + J_{-\nu}(\xi)]$$

$$\mathcal{B}i_\nu(-x) = \nu^{1/2}\ x^{1/2}[I_{-\nu}(\xi) + I_\nu(\xi)]$$

$$\mathcal{B}i_\nu(x) = \nu^{1/2}\ x^{1/2}[J_{-\nu}(\xi) - J_\nu(\xi)] \qquad (14).$$

where, as defined before, $\xi = 2c\nu\ x^{\frac{1}{2\nu}}$. The multiplicative factors have been picked to make the Wronskian W of the generalized Airy functions the same as for the usual Airy functions

$$W\{\mathcal{A}i_\nu(x)\ ,\ \mathcal{B}i_\nu(x)\} \equiv \mathcal{A}i_\nu(x)\frac{d}{dx}\mathcal{B}i_\nu(x) - \mathcal{B}i_\nu(x)\frac{d}{dx}\mathcal{A}i_\nu(x) = \pi^{-1} \qquad (15)$$

The generalized Airy functions, of course, obey the same type of relations that the Ai and Bi functions do. In particular, the identity

$$\mathcal{B}i_\nu(x) = e^{(\pi i/2-\pi\nu i)}\,\mathcal{A}i_\nu[xe^{(2\pi\nu i)}] + e^{(\pi\nu i-\pi i/2)}\mathcal{A}i_\nu[xe^{(-2\pi\nu i)}] \qquad (16)$$

is operative. The series expansions for these generalized functions are readily obtained from the series representations of the Bessel functions.

Gordon[2] has recently calculated the Ai and Bi functions to great accuracy using the method of generalized Gaussian quadrature. In order to apply this method to the calculation of the $\mathcal{A}i_\nu$ and $\mathcal{B}i_\nu$ functions, it is necessary to express them in terms of the Bessel function of imaginary argument $K_\nu(z) = \frac{1}{2}\pi\csc(\nu\pi)[I_{-\nu}(z) - I_\nu(z)]$. Using the identity[7]

$$K_\nu(u) = \pi^{-1}\cos(\nu\pi)\, u^{1/2} \quad e^{-u}\int_0^\infty \frac{e^{-x}K_\nu(x)}{x^{1/2}(x+u)}\,dx \tag{17}$$

and Eq. (16), the pair of relations are obtained:

$$\mathcal{A}i_\nu(-x) = \frac{1}{2}\cos(\nu\pi)\pi^{-3/2}\, c^{-1/2}\, x^{1/2-1/4\nu} \quad e^{-\xi}\int_0^\infty \frac{\rho(u)}{1+(u/\xi)}\,du$$

$$\mathcal{B}i_\nu(-x) = \cos(\nu\pi)\pi^{-3/2}\, c^{-1/2}\, x^{1/2-1/4\nu} \quad e^{+\xi}\int_0^\infty \frac{\rho(u)}{1-(u/\xi)}\,du$$

(18)

where

$$\rho(u) = (2/\pi)^{1/2}\, u^{-1/2} \quad e^{-u}\, K_\nu(u) \tag{19}$$

and c in the constant in Eq. (1).*

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* Unfortunately, Gordon's Eq. (A9) has a typographical error. It should read

$$\rho(x) = 2^{-1/2}\,\pi^{-3/2}\,x^{-1/2} \quad e^{-x}\,K_{1/3}(x) \quad .$$

Using this equation, his Eq. (A10) is obtained. Also his Eqs. (A14) and (A15) are wrong. However, Eqs. (A16) and (A17) are correct.

In terms of K_ν , the generalized Airy functions for positive x are:

$$\mathcal{A}i_\nu(x) = i/2\ \pi^{-1} \csc(\nu\pi/2)\ \nu^{1/2}\ x^{1/2}\ [K_\nu(i\xi) - K_\nu(-i\xi)]$$

$$\mathcal{B}i_\nu(x) = 2\pi^{-1} \sin(\nu\pi/2)\ \nu^{1/2}\ x^{1/2}\ [K_\nu(i\xi) + K_\nu(-i\xi)] \quad . \tag{20}$$

The corresponding integral expressions are given by

$$\mathcal{A}i_\nu(x) = \frac{1}{2}\, c^{-1/2}\pi^{-3/2} \csc(\nu\pi/2)\cos(\nu\pi)\ x^{1/2-1/4\nu} \int_0^\infty \frac{\cos(\xi-\pi/4) + (u/\xi)\sin(\xi-\pi/4)}{1 + (u/\xi)^2}\, \rho(u)\, du$$

$$\mathcal{B}i_\nu(x) = 2c^{-1/2}\ \pi^{-3/2} \sin(\nu\pi/2)\cos(\nu\pi)\ x^{1/2-1/4\nu} \int_0^\infty \frac{(u/\xi)\cos(\xi-\pi/4) - \sin(\xi-\pi/4)}{1 + (u/\xi)^2}\, \rho(u)\, du \tag{21}$$

where $\rho(u)$ is the same as Eq. (19).

The moments, μ_k , of the positive function $\rho(u)$ can be found using the identity[8]

$$\int_0^\infty x^{j-1}\ e^{-x}\ K_\nu(x)dx = \pi^{-1/2}\ 2^{-j}\ \frac{\Gamma(j+\nu)\Gamma(j-\nu)}{\Gamma(j+1/2)} \tag{22}$$

Thus,

$$\mu_k = \int_0^\infty x^k \rho(x)dx = \frac{\Gamma(k + 1/2 + \nu)\,\Gamma(k + 1/2 - \nu)}{2^k\, k!} \tag{23}$$

Using the μ_k , the integral expressions for the generalized Airy functions can be approximated as sums of n points and n weights determined by a generalized Gaussian quadrature algorithm given elsewhere.[9]

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