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Schrödinger Equation Solutions for small r and resulting Functional Relations

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Abstract

The Schrödinger equation is examined for small r (i.e. one step beyond the limit $r \to 0$) for the cases $V(r) \to r^k$, $(k > 0)$, and $V(r) \to r^{-k}$ $(0 < k < 2)$. In both cases the solutions are related to appropriate Bessel functions. This result may be used to obtain approximate functional relations involving Bessel functions. One such relation is derived in detail and illustrated graphically.

Key Words: Schrödinger equation, Bessel equation, Airy functions, Associated Laguerre functions

Consider first the Schrödinger equation for the attractive potential (or more generally for any potential that goes as r^k for small r):

$$V(r) = Ar^k, \quad k > 0: \tag{1}$$

$$\left[-\frac{1}{2}\left(\frac{d^2}{dr^2} - \frac{l(l+1)}{r^2}\right) + Ar^k\right] u_{nl}(r) = E u_{nl}(r). \tag{2}$$

To get the $r \to 0$ limit for the wavefunction $u_{nl}(r)$, the usual procedure [1] is to examine only the first two terms of this equation, namely for $r \to 0$

$$-\frac{1}{2}\left(\frac{d^2}{dr^2} - \frac{l(l+1)}{r^2}\right) u_{nl}(r) = (E - Ar^k) u_{nl}(r) \sim 0 \tag{3}$$

i.e.

$$u_{nl}(r) \sim F r^{l+1}, \tag{4}$$

(rejecting the other solution Gr^{-l} that blows up at the origin.)

For the case $k > 0$ one can clearly go beyond this approximation to somewhat larger r by also including the energy term, i.e:

$$\left[-\frac{1}{2}\left(\frac{d^2}{dr^2} - \frac{l(l+1)}{r^2}\right) - E\right] u_{nl}(r) = -Ar^k u_{nl}(r) \sim 0, \tag{5}$$

which, when compared to the spherical Bessel equation for $rj_l(r)$

$$\left(\frac{d^2}{dr^2} - \frac{l(l+1)}{r^2} + 1\right) rj_l(r) = 0 \tag{6}$$

is immediately seen to have the solution:

$$u_{nl}(r) \sim Crj_l\left(\sqrt{2E}r\right) = Cr^{1/2}\sqrt{\frac{\pi}{2}}J_{l+1/2}\left(\sqrt{2E}r\right) \tag{7}$$

For $r \to 0$ [2],

$$j_l(r) = \frac{r^l}{(2l+1)!!}\left\{1 - \frac{r^2/2}{2l+3} + ...\right\} \sim \frac{r^l}{(2l+1)!!} \tag{8}$$

i.e., as required this more general result, eq. (7), reduces to eq. (4) in the limit $r \to 0$.

It is of interest to observe eq. (7) that gives the form of the wavefunction for small r (an expression that depends on E, though not on A or k), can also be used to obtain approximate functional relations.

Thus, if $k = 2,\ A = 1/2$, eq. (2) involves the simple harmonic oscillator system with $n = 0, 1, ..,\ E = 2n + l + 3/2$, and exact solutions:

$$u_{nl}(r) \sim r^{l+1}e^{-r^2/2}{}_1F_1(-n; l+3/2; r^2) \to r^{l+1} \quad \text{as } r \to 0.$$

These oscillator wavefunctions can be related to the Bessel functions via eq. (7), i.e. $u_{nl}(r) \sim Crj_l(\sqrt{4n+2l+3}\ r)$. To obtain the constant C in eq. (7) for this case, one notes that for the simple harmonic oscillator wavefunction, $u_{nl}(r) \to_{r\to 0} r^{l+1}$ and using eq. (8), as $r \to 0$,

$$u_{nl}(r) \to r^{l+1} \sim Crj_l(\sqrt{2E}r) \to \frac{Cr(\sqrt{2E}r)^l}{(2l+1)!!}, \quad \text{i.e.} \quad C = \frac{(2l+1)!!}{(\sqrt{2E})^l} \ .$$

Redefining $\sqrt{2E}\ r \to r$, and noting that for this potential $E = 2n + l + 3/2$, one has:

$$j_l(r) = \sqrt{\frac{\pi}{2r}}J_{l+1/2}(r) \sim \frac{r^l}{(2l+1)!!}e^{-r^2/(8n+4l+6)}{}_1F_1(-n; l+3/2; r^2/(4n+2l+3)) \ . \tag{9}$$

This formula can also be obtained using an expression [3] for the Bessel function in terms of Associate Laguerre functions. It is very accurate for small r as can be seen from figures 1 and 2. These figures were drawn using the Mathematica software [4].

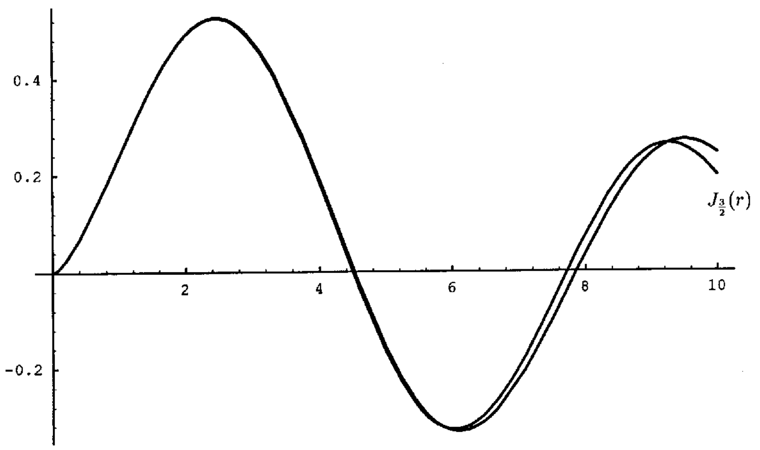

Figure 1. Plot for $n = 5$, and $l = 1$, of

$$J_{l+1/2}(r) \quad \text{and} \quad \sqrt{\frac{2}{\pi}} \frac{r^{l+\frac{1}{2}}}{(2l+1)!!} e^{-r^2/(8n+4l+6)} \,{}_1F_1\Big(-n; l+\frac{3}{2}; r^2/(4n+2l+3)\Big)$$

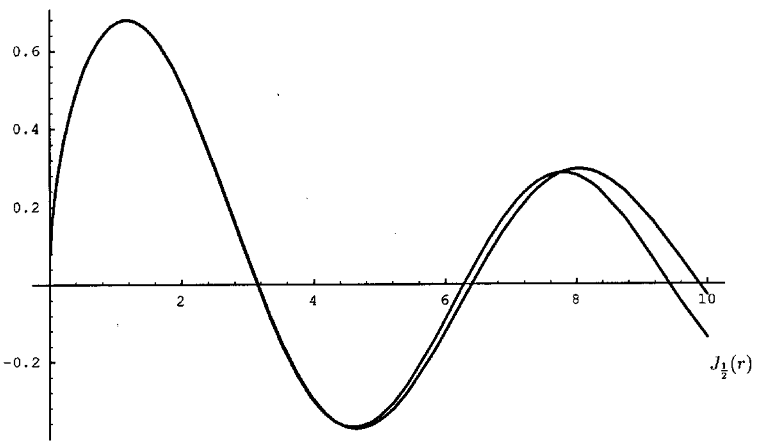

Figure 2. Plot for $n = 4$, and $l = 0$, of

$$J_{l+1/2}(r) \quad \text{and} \quad \sqrt{\frac{2}{\pi}} \frac{r^{l+\frac{1}{2}}}{(2l+1)!!} e^{-r^2/(8n+4l+6)} \,{}_1F_1\Big(-n; l+\frac{3}{2}; r^2/(4n+2l+3)\Big)$$

If both sides of eq. (9) are expanded in powers of r, one can easily verify that the first two terms are equal.

If one examines the case $k = 1$, one can similarly relate the Bessel and Airy functions, etc.

This procedure (and hence eq. (7)) cannot be applied to potentials where $k < 0$, (i.e. when the potential goes as $r^{-|k|}$ as $r \to 0$) since the r.h.s. of eq. (5) is not small in this limit. However, if one considers the three-dimensional Schrödinger equation for an attractive potential that goes as r^{-k}:

$$V(r) = -|A| r^{-k} \qquad 0 < k < 2,$$

$$\left[-\frac{1}{2}\left(\frac{d^2}{dr^2} - \frac{l(l+1)}{r^2}\right) - |A| r^{-k} - E\right] u_{nl}(r) = 0, \tag{10}$$

and applies the transformation [5,6] $r = \rho^m, \quad m = 2/(2-k)$, this yields the "related" Schrödinger equation:

$$\left[-\frac{1}{2}\left(\frac{d^2}{d\rho^2} - \frac{(k_m - 1)(k_m - 3)}{4\rho^2}\right) - \frac{4|A|}{(2-k)^2}\right] w^m(\rho) = \frac{4E}{(2-k)^2} \rho^{\frac{2k}{2-k}} w^m(\rho), \tag{11}$$

where $k_m = (4l + 6 - 2k)/(2-k), \quad u_{nl}(r) = \rho^{(m-1)/2} w^m(\rho)$. For small ρ one can ignore the term on the r.h.s. of eq. (11).

Thus, if $K \equiv \frac{\sqrt{8|A|}}{(2-k)}, \quad y = K\rho$, for small ρ this equation becomes:

$$\left(\frac{d^2}{dy^2} - \frac{(k_m - 1)(k_m - 3)}{4y^2} + 1\right) w^m(y) \sim 0, \tag{12}$$

which one can again compare with the Bessel differential eq. (6).

Hence, in this case one obtains finally for small r:

$$u_{nl}(r) \sim C r^{1-\frac{k}{4}} \, j_{\frac{4l+k}{2(2-k)}}\left(\frac{\sqrt{8|A|}}{2-k} r^{(2-k)/2}\right) \ . \tag{13}$$

This result is independent of E, but depends on $|A|$, and k. Additionally, as it should, for $r \to 0$ it too reduces to eq. (4).

Consider for example the Coulomb potential system ($k = 1, \ m = 2, \ |A| = 1$). For small r eq. (13) implies one can also relate Coulomb and Bessel functions. For this case:

$$u_{nl}(r) \sim C r^{3/4} j_{2l+1/2}\left(\sqrt{8}\, r^{1/2}\right) = C\sqrt{\frac{\pi}{2}}\, r^{1/4} J_{2l+1}\left(\sqrt{8}\, r^{1/2}\right). \tag{14}$$

Conclusion

For potentials that go as Ar^k ($k > 0$), or Ar^{-k} ($0 < k < 2$), for small r the solutions of the Schrödinger equation can be related to specific Bessel functions. In the former case the relation(eq. (7)) involves E, and in the latter(eq. (13)), A, and k. For the special cases where the exact solutions are known analytically, this leads to approximate functional relations between these solutions and appropriate Bessel functions. In particular this discussion explains why and how Bessel, and harmonic oscillator, Airy, Coulomb, etc. functions are related for small r. The relation obtained for the harmonic oscillator case is discussed in detail and illustrated graphically.

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References

[1] E. Merzbacher, J. Wiley 2nd edition 1971 p. 201.

[2] Handbook of Mathematical Functions Eds Abramowitz & Stegun p. 437.

[3] Erdélyi, Higher Transcendental Functions v. 2, p. 199.

[4] S. Wolfram, Mathematica, (Addison-Wesley Publishing Company, 1988).

[5] H. A. Mavromatis, "Families of Interrelated Schrödinger Equations", *J. Phys. A* **30**, pp. 1685-1688 (1997).

[6] H. A. Mavromatis, "Transformations between Schrödinger Equations", *Am. J. Phys.* **66** (1998) pp. 335-337.