ON AN INTEGRAL IN THE DISTRIBUTION OF EIGENVALUES

by J. B. McLEOD

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1. In the case of a wave function with spherical symmetry, the wave equation can be separated using spherical polar coordinates, and the equation for the radial component becomes

$$\frac{d^2\psi}{dr^2}+\left\{\lambda-q(r)-\frac{l(l+1)}{r^2}\right\}\psi=0, \qquad \text{(1.1)}$$

where λ is a constant parameter, proportional to the energy of the particle under consideration, $q(r)$ is proportional to the potential energy, and l is a positive integer or zero.

In a recent paper (**1**) I discussed the distribution of the eigenvalues for cases of (1.1) similar to that of the hydrogen atom, for which $q(r)$ is proportional to $-1/r$. To make this situation analytically precise, we set

$$V(r) = q(r)+(l+\tfrac{1}{2})^2/r^2$$

and impose the following conditions on $V(r)$ and $q(r)$:

(i) except at $r = 0$, $q(r)$ is continuously differentiable, while, as $r\to 0$, $q(r) = O(r^{-2+c})$ for some fixed $c>0$;

(ii) $V(r)$ has one and only one zero, and that simple, from which it follows that $V(r)<0$, $q(r)<0$ for sufficiently large r;

(iii) as $r\to\infty$, $V(r)$ is three times continuously differentiable, and $V(r)\to 0$ with

$$\frac{V'(r)}{-V(r)}\asymp\frac{1}{r},\ \frac{V''(r)}{V'(r)}=O\left(\frac{1}{r}\right),\quad \frac{V'''(r)}{V'(r)}=O\left(\frac{1}{r^2}\right),$$

where $\asymp$ means that the ratio of the two sides lies between positive constants;

(iv) as $r\to\infty$, $r^{d-2}\{-V(r)\}^{-1}$ is a decreasing function for some fixed $d>0$.

If we now impose on solutions of (1.1) the boundary condition that they be $L^2(0, \infty)$ (or, if $l = 0$, that in addition they vanish at the origin), then we will have defined an eigenvalue problem which will have a discrete spectrum for $\lambda<0$ and a continuous spectrum for $\lambda>0$. (These results are proved in (**1**)). In § 6 of (**1**), I obtained a formula for the distribution of the discrete eigenvalues for which we require the following notation.

From (i) and (ii) above, we have that for λ_n sufficiently small and negative, $\lambda_n - V(r)$ has exactly two zeros, one being close to the zero of $V(r)$ while the other tends to infinity as $\lambda_n \to 0$. We therefore define R_2 to be the smaller zero of $\lambda_n - V(r)$, r_1 to be the zero of $V(r)$, and $q(\lambda)$ to be the inverse function to $V(r)$ for large r, with $q(\lambda_n) = q_n$; thus q_n is the larger zero of $\lambda_n - V(r)$. We finally define

$$\omega = \omega(r) = \tan^{-1}\left\{[-V(r)]^{\frac{1}{2}}[r^{-\frac{1}{2}}V_1(r)] \Big/ \frac{d}{dr}[r^{-\frac{1}{2}}V_1(r)]\right\},$$

where $V_1(r)$ is the solution of (1.1) with $\lambda = 0$ which vanishes at the origin, the existence and uniqueness (apart from an unimportant constant factor) of this function being guaranteed by Lemma 3(a) of (**1**); the correct branch of the inverse tangent is determined by insisting that $\omega(r_1) = 0$ and that ω be continuous.

We then have the result that the $(n+1)$th eigenvalue λ_n, as we approach zero through negative values, is given by

$$(n+\tfrac{3}{4})\pi = \int_{R_2}^{q_n} \{\lambda_n - V(r)\}^{\frac{1}{2}} dr + \tfrac{1}{4}\int_{r_1}^{\infty} \frac{d/dr[r^2V(r)]}{r^2V(r)} \sin 2\omega \, dr + O\{\lambda_n^{\frac{1}{2}}V^{-\frac{1}{2}}[(-\lambda_n)]^{-\frac{1}{2}}\}. \quad \text{......(1.2)}$$

The usual approximation of the physicist to this is

$$(n+\tfrac{1}{2})\pi = \int_{R_2}^{q_n} \{\lambda_n - V(r)\}^{\frac{1}{2}} dr, \quad \text{......(1.3)}$$

where the size of the error involved is not specified. If, however, it is understood (as seems reasonable) that the error tends to zero, as $n \to \infty$, then, in order for (1.2) and (1.3) to be consistent, the second integral in (1.2) (which is a constant independent of n) must take the value π. In fact, it is surprising (but true) that the integral does take the value π if $q(r)$ takes the special form $-kr^{-a}$ $(0<a<2)$, k being some positive constant. This is proved in § 6 of (**1**).

The question then arises whether this is in the nature of a freak result or whether it is true for all $q(r)$ satisfying the conditions of the theorem. It is the purpose of this note to show that the first alternative is the case by demonstrating a function $q(r)$ for which the integral does not take the value π.

2. By (6.4) of (**1**), we have

$$\int_{r_1}^{\infty} \frac{d/dr[r^2V(r)]}{r^2V(r)} \sin 2\omega \, dr = \lim_{R\to\infty} 4\left\{\omega(R) - \int_{r_1}^{R} [-V(r)]^{\frac{1}{2}} dr\right\}. \quad \text{...(2.1)}$$

In the case where $q(r) = -kr^{-a}$, we can, as in (**1**), evaluate the right-hand side of (2.1) and so show that the left-hand side has the required value π. We now want to show that we can alter $q(r)$ away from $-kr^{-a}$ and by so doing alter the right-hand side (and so the left-hand side) of (2.1).

Consider therefore $q(r)$ changed from $-kr^{-a}$ to a function $q^*(r)$ satisfying

$$q^*(r) = -kr^{-a} \quad \text{for} \quad \tfrac{1}{2}r_1 \leq r < \infty \quad \text{......(2.2)}$$

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but being otherwise at present undefined, except that it must continue to satisfy the general conditions (i)-(iv) of § 1. It should be remarked that with this definition r_1 is unaltered by the change in $q(r)$, so that there is no danger of confusion as to which value of r_1 is meant in (2.2).

Then the integral on the right-hand side of (2.1) is unaltered by the change in $q(r)$, and so whether the right-hand side or left-hand side is altered depends upon whether $\omega(R)$ is altered.

Now the general solution of the equation

$$\frac{d^2\psi}{dr^2} - \left\{q^*(r) + \frac{l(l+1)}{r^2}\right\}\psi = 0$$

for $\frac{1}{2}r_1 \leqq r < \infty$ is (as in (1), § 6)

$$Ar^{\frac{1}{2}}J_\beta(\xi) + Br^{\frac{1}{2}}J_{-\beta}(\xi),$$

where A, B are arbitrary constants and

$$\beta = (2l+1)/(2-a), \quad \xi = 2k^{\frac{1}{2}}r^{1-\frac{1}{2}a}/(2-a).$$

We can certainly arrange the uncommitted part of $q^*(r)$ so that the solution $V_1(r)$ which vanishes at $r = 0$ satisfies the condition $B \neq 0$. This will be as far as we need define $q^*(r)$.

Then, as $r \to \infty$, we have from the well-known asymptotic formulæ for Bessel functions that for some A, B, with $B \neq 0$,

$$V_1(r) = Ar^{\frac{1}{2}}\left(\frac{2}{\pi\xi}\right)^{\frac{1}{2}}[\cos(\xi - \tfrac{1}{2}\beta\pi - \tfrac{1}{4}\pi) + O(\xi^{-1})] +$$
$$+ Br^{\frac{1}{2}}\left(\frac{2}{\pi\xi}\right)^{\frac{1}{2}}[\cos(\xi + \tfrac{1}{2}\beta\pi - \tfrac{1}{4}\pi) + O(\xi^{-1})],$$

with a corresponding formula for $V_1'(r)$ which is obtained from the above by formal differentiation. To simplify the resulting arithmetic, let us suppose specifically that $l = 0$, $a = \frac{4}{3}$, $\beta = \frac{3}{2}$. Then, if we substitute the expressions for $V_1(r)$, $V_1'(r)$ in the definition of $\omega(r)$ in § 1, we obtain that

$$\omega(r) = \tan^{-1}\left\{-\frac{[-V(r)]^{\frac{1}{2}}[-A\cos\xi - B\sin\xi + O(\xi^{-1})]}{k^{\frac{1}{2}}r^{-\frac{1}{2}a}[-A\sin\xi + B\cos\xi + O(\xi^{-1})]}\right\}.$$

Let us sufficiently put $A = \cos\eta$, $B = \sin\eta$, so that

$$\omega(r) = \tan^{-1}\left\{-\frac{[-V(r)]^{\frac{1}{2}}[\cos(\xi - \eta) + O(\xi^{-1})]}{k^{\frac{1}{2}}r^{-\frac{1}{2}a}[\sin(\xi - \eta) + O(\xi^{-1})]}\right\}$$
$$= \xi - \eta + \tfrac{1}{2}\pi \pm m\pi + o(1), \quad \text{as } r \to \infty,$$

where m is some positive integer or zero.

If $B = 0$, which occurs when $q(r) = -kr^{-a}$ for all r, we have

$$\omega(r) = \xi + \tfrac{1}{2}\pi \pm m'\pi + o(1), \text{ as } r \to \infty,$$

where m' is also some positive integer or zero. Hence the change in $\omega(R)$ in (2.1), when we change $q(r)$ from $-kr^{-a}$ to $q^*(r)$, is, as $R \to \infty$,

$$\pm(m'-m)\pi+\eta+o(1).$$

Since $B \neq 0$ for $q^*(r)$, η is not a multiple of π, and so there will be a non-zero change in the right-hand side of (2.1), and so also in the left-hand side.

This completes the construction of the necessary example.

REFERENCE

(1) J. B. McLeod, The distribution of the eigenvalues for the hydrogen atom and similar cases, *Proc. London Math. Soc.* (3), **11** (1961), 139-158.

Wadham College
Oxford