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Comments on the one-dimensional hydrogen atom [Am. J. Phys. 27, 649 (1959); Am. J. Phys. 37, 1145 (1969); Am. J. Phys. 44, 1064 (1976)

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It sometimes happens that extraneous solutions are introduced in a problem that must be explained away by some mathematical or physical argument. A well-known example occurs in electrostatics when solving

$$\nabla^2 V = 0$$

in spherical coordinates. Here $V \sim 1/r$ is apparently a solution. However, it is a solution only for $r \neq 0$, and, as is well known, is in fact the potential due to a point charge located at the origin,

$$\nabla^2(1/r) = -4\pi\delta(\mathbf{r}).$$

No such singularity arises when attacking the problem in Cartesian coordinates.

The purpose of this note is to show that the controversial solutions[1–5] to the Schrödinger equation for the one-dimensional hydrogen atom fall into the category of extraneous solutions, similar to the above example. These solutions do not satisfy the Schrödinger equation at the origin, and, furthermore, given any two such solutions, ψ and $\tilde{\psi}$,

$$\left| \int_{-\infty}^{\infty} dx\, \psi^{+} (H-E) \tilde{\psi} \right| \to \infty,$$

where H is the appropriate Hamiltonian and E is its eigenvalue. Thus no measurable spectrum exists and these solutions must be disregarded.

To prove this assertion, consider the one-dimensional Schrödinger equation ($m = \hbar = 1$)

$$H\Psi = E\Psi \tag{1}$$

with

$$H = -\frac{1}{2}\frac{d^2}{dx^2} - \frac{\lambda}{|x|}; \quad E = -\frac{k^2}{2}.$$

Because of the singularity at the origin, solutions must be obtained separately for regions $x > 0$ and $x < 0$ and then matched appropriately at $x = 0$. The solutions[6] for the even extensions are

$$\Psi_1 = A_1 |x| e^{-k|x|} M(1-\lambda/k, 2, 2k|x|) \tag{2a}$$

and

$$\Psi_2 = A_2 e^{-k|x|} U(-\lambda/k, 0, 2k|x|), \tag{2b}$$

where A_1 and A_2 are normalization constants and M and U are the regular and irregular confluent hypergeometric functions defined on p. 504 of Ref. 6. These solutions are linearly dependent for the special cases, where λ/k is a positive integer. The odd extensions are given by

$$\Psi_{3,4} = \operatorname{sgn} x\, \Psi_{1,2}.$$

The wavefunction Ψ_1 satisfies the boundary condition at $|x| \to \infty$ only if M is a polynomial, i.e., only if $\lambda/k = n$; $n = 1, 2$, the usual spectrum of the three-dimensional hydrogen atom in the case of zero angular momentum.

The wavefunction Ψ_2, however, automatically satisfies the boundary condition at $|x| \to \infty$. Moreover, it is Lebesque square integrable and continuous at $x = 0$. It is these "solutions" that are controversial since they apply for all values of k; a result that implies a negative energy continuum.[2] Or if the potential is replaced by

$$V = \lim_{a \to 0} \frac{-\lambda}{|x| + a},$$

a ground state at $E = -\infty$ is obtained with the corresponding eigenfunction, in the limit $a \to 0 (|k| \to \infty)$ for small x,

$$\Psi_2 = (k)^{1/2} e^{-k|x|}, \tag{3a}$$

where a and k satisfy

$$\ln 2ak + \frac{\Gamma'(1-\lambda/k)}{\Gamma(1-\lambda/k)} = 0. \tag{3b}$$

This state is not required for completeness in the expansion of square integrable functions.[3] Here $\Gamma(1+z) = z\Gamma(z)$ is the gamma function and $(d/dz)\Gamma(z) = \Gamma'(z)$.

The controversy arises because $\Psi_{1,2,4}$ are not solutions of Eq. (1). For example, the even extensions $\Psi_{1,2}$ satisfy

$$-\frac{1}{2}\frac{d^2\Psi_{1,2}}{d|x|^2} - \frac{\lambda}{|x|}\Psi_{1,2} = -\frac{k^2}{2}\Psi_{1,2} \tag{4}$$

rather than Eq. (1). To see the difference use

$$\frac{d^2}{dx^2} = \left(\frac{d|x|}{dx}\right)^2 \frac{d^2}{d|x|^2} + \frac{d^2|x|}{dx^2}\frac{d}{d|x|} \tag{5a}$$

with[7]

$$|x| = x \operatorname{sgn} x \text{ and } \frac{d}{dx}\operatorname{sgn} x = 2\delta(x)$$

to give

$$\frac{d^2}{dx^2} = (\operatorname{sgn} x + 2x\delta^2(x) \frac{d^2}{d|x|^2} + 2[2\delta(x) + x\delta'(x)]\frac{d}{d|x|}, \tag{5b}$$

where the prime denotes the derivative. Then for $\Psi = \Psi_{1,2}$, Eq. (1) becomes

$$(H-E)\Psi_{1,2} = -2[|x|\delta(x) + x^2\delta^2(x)]\left(k^2 - \frac{2\lambda}{|x|}\right)\Psi_{1,2} - [2\delta(x) + x\delta'(x)]\frac{d\Psi_{1,2}}{d|x|}. \tag{6}$$

Near the origin,[6]

$$\Psi_1 = A_1 k |x| (1 - \lambda |x|) + 0(|x|^3);$$

$$\Psi_2 = \frac{A_2}{\Gamma(1-\lambda/k)} + 0(|x| \ln |x|);$$

and

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$$\Psi_2' = -\frac{A_2 k}{\Gamma(1-\lambda/k)} \times\left[1+2\frac{\lambda}{k}\left(\ln 2k|x| + \frac{\Gamma'(1-\lambda/k)}{\Gamma(1-\lambda/k)}\right)\right] + 0(|x|\ln|x|). \quad (7)$$

For Ψ_1, Eq. (6) becomes

$$(H-E)\Psi_1 = -A_1 k\delta(x) \quad (8)$$

and for Ψ_2

$$(H-E)\Psi_2 = \frac{\lambda A_2}{\Gamma(1-\lambda/k)} \times\left[\left(4+k/\lambda+2\frac{\Gamma'(1-\lambda/k)}{\Gamma(1-\lambda/k)}\right)\delta(x) + 2\ln(2k|x|)[2\delta(x)+x\delta'(x)]\right]. \quad (9)$$

Clearly, neither Ψ_1 nor Ψ_2 satisfies Eq. (1) at the origin. However, Ψ_1 is equivalent to a solution of Eq. (1), since given any two Ψ_1's, say Ψ_1 and $\widetilde{\Psi}_1$,

$$\int dx\, \Psi_1^\dagger\, (H-E)\widetilde{\Psi}_1 = 0. \quad (10)$$

This argument fails for Ψ_2 as can be seen by examination of Eqs. (7) and (9),

$$\int dx\, \Psi_2^\dagger\, (H-E)\widetilde{\Psi}_2 \to \infty. \quad (11)$$

A similar analysis of the odd extensions $\Psi_{3,4}$ gives for the regular function Ψ_3,

$$(H-E)\Psi_3 = 0, \quad (12)$$

whereas for the irregular solution Ψ_4,

$$\int \Psi_4^\dagger\, (H-E)\widetilde{\Psi}_4\, dx \to \infty. \quad (13)$$

Thus the appropriate solutions to Eq. (1) are the even and odd extensions of the regular solution $\Psi_{1,3}$.

A regular solution ($\Psi/x\to A, \Psi'\to A$ as $x\to 0$) can always be found[8] for singular potentials that satisfy $\lim_{x\to 0} x^2 V(|x|)\to 0$. Application of the above analysis shows that the even extensions of such solutions are acceptable. For potentials that also satisfy $\lim_{x\to 0}|x|V(|x|)\to 0$, there exist irregular solutions $\Psi\to\text{const}$, $\Psi'\to 0$, for $x\to 0$. The even extensions of such solutions are also acceptable solutions to the Schrödinger equation. On the other hand, for $\lim_{x\to 0}|x|V(|x|)\nrightarrow 0$ the irregular solution satisfies $\Psi'\to\infty$ for $x\to 0$ as in the case of the Coulomb potential. Thus these irregular solutions must be discarded.

The scattering solution for an incoming wave $e^{-ikx}, x\geqslant 0$; e^{ikx}, $x\leqslant 0$, can be obtained for the Coulomb potential from Eq. (2a) by replacing k by $\pm ik$,

$$\Psi = Axe^{-ikx}M[1-(\lambda/ik),2,2ikx]; \quad x\geqslant 0,$$
$$= Axe^{ikx}M[1-(\lambda/ik),2,-2ikx]; \quad x\geqslant 0, \quad (14)$$

which for large x becomes[6]

$$\Psi\to -\frac{e^{\mp\pi\lambda/2k}A}{\Gamma(1\pm\lambda/ik)}\left(e^{\mp ikx}e^{\mp i(\lambda/k)\ln 2k|x|} - \frac{\Gamma(1\pm\lambda/ik)}{\Gamma(1\mp\lambda/ik)}e^{\pm ibx}e^{\pm i(\lambda/k)\ln 2k|x|}\right). \quad (15)$$

The reflection coefficient is

$$R = \left|\frac{\Gamma(1\pm\lambda/ik)}{\Gamma(1\mp\lambda/ik)}\right|^2 = 1. \quad (16)$$

Thus the potential $V = -\lambda/|x|$ divides the configuration space into two independent halves as first noted by Andrews.[4]

Note also that the bound state solutions $\Psi_{1,3}$ for each half, $x\geqslant 0$ and $x\leqslant 0$, can be recovered by a contour integration[9] that encircles the poles of the continuum wavefunction [Eq. (14)] that for $x>0$ are at $\lambda/ik = -n$, $n = 1, 2,...$ and for $x\leqslant 0$ are at $\lambda/ik = n$.

We therefore conclude that the appropriate solutions to the one-dimensional hydrogen atom are the even and odd extensions of the regular functions $\Psi_{1,3}$ and that the irregular functions $\Psi_{2,4}$ must be discarded since they neither satisfy the Schrödinger's equation over the entire domain of x nor do they give rise to a definable energy spectrum. This resolves the controversy since the solutions posed in Refs. 1 and 2 fall into this irregular category.

Note that Loudon's solution [Eq. (3)] is a solution of the free particle Schrödinger equation

$$\frac{-d^2}{2\,dx^2}\psi = -\frac{k^2\psi}{2},$$

rather than the solution to Eq. (1). He has therefore, in this limiting process, thrown away the effect of the irregular nature of the potential. He has a result that would apply equally well to the free particle case, i.e., a bound state at $E = -\infty$ for the free particle with Eq. (3) as its eigenfunction.

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