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Critique and correction of the currently accepted solution of the infinite spherical well in quantum mechanics

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Abstract – An error in the currently accepted solution of the problem of the infinite spherical well is pointed out. The problem is then solved by considering the self-adjointness of the Hamiltonian operator. In contrast to the currently accepted solution, the radial probability density for finding the particle at the center of the spherical well is not necessarily zero, in accordance with the solutions obtained.

The currently accepted solution of the infinite spherical well. – The usual way of solving the problem of the infinite spherical well is recapitulated in the following [1–3]. Consider a particle of mass μ being confined in a well of spherically symmetric potential

$$V(r) = \begin{cases} 0, & \text{if } r \le a, \\ \infty, & \text{if } r > a. \end{cases} \tag{1}$$

The time-independent Schrödinger wave equation for the system is

$$\hat{H}\psi(\mathbf{r}) = \left[-\frac{\hbar^2}{2\mu}\bigtriangledown^2 + V(r)\right]\psi(\mathbf{r}) = E\psi(\mathbf{r}). \tag{2}$$

In terms of the spherical coordinates (r, θ, ϕ), the equation becomes

$$\frac{1}{2\mu r^2}\left[-\hbar^2\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right) + \hat{\mathrm{L}}^2\right]\psi + V(r)\psi = E\psi. \tag{3}$$

Here, the operator $\hat{\mathrm{L}}^2$ is the square of the angular momentum operator $\hat{\mathbf{L}}$,

$$\hat{\mathrm{L}}^2 = -\hbar^2\left[\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right) + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2}\right]. \tag{4}$$

By the separation of variables, substituting $\psi(r, \theta, \phi) = R(r)Y(\theta, \phi)$ into eq. (3) yields the angular equation

$$\frac{1}{Y}\left\{\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial Y}{\partial\theta}\right) + \frac{1}{\sin^2\theta}\frac{\partial^2 Y}{\partial\phi^2}\right\} = -l(l+1), \tag{5}$$

and the radial equation

$$-\frac{\hbar^2}{2\mu r^2}\frac{\mathrm{d}}{\mathrm{d}r}\left(r^2\frac{\mathrm{d}R}{\mathrm{d}r}\right) + \left[V(r) + \frac{\hbar^2 l(l+1)}{2\mu r^2}\right]R = ER. \tag{6}$$

The solutions of eq. (5) are spherical harmonics:

$$Y_l^m(\theta,\phi) = (-1)^{(m+|m|)/2} \times\sqrt{\frac{2l+1}{4\pi}\frac{(l-|m|)!}{(l+|m|)!}}P_l^m(\cos\theta)e^{i\,m\phi}, \tag{7}$$

where $l = 0, 1, 2, 3, \ldots$, $m = -l, \ldots, l$ in integer steps, and $P_l^m(\cos\theta)$ are associated Legendre functions. These spherical harmonics are common eigenstates of the operators $\hat{\mathrm{L}}^2$ and $\hat{\mathrm{L}}_z$, *i.e.*, $\hat{\mathrm{L}}^2 Y_l^m = l(l+1)\hbar^2 Y_l^m$ and $\hat{\mathrm{L}}_z Y_l^m = m\hbar Y_l^m$. They are orthonormal,

$$\int_{\phi=0}^{2\pi}\int_{\theta=0}^{\pi}[Y_l^m(\theta,\phi)]^*[Y_{l'}^{m'}(\theta,\phi)]\sin\theta\,\mathrm{d}\theta\,\mathrm{d}\phi = \delta_{ll'}\delta_{mm'}. \tag{8}$$

Outside the well $V(r) = \infty$, thus the radial wave function $R(r) = 0$ for $r > a$. Inside the well $V(r) = 0$, thus eq. (6) becomes

$$\frac{\mathrm{d}^2R}{\mathrm{d}r^2} + \frac{2}{r}\frac{\mathrm{d}R}{\mathrm{d}r} + \left[k^2 - \frac{l(l+1)}{r^2}\right]R = 0, \tag{9}$$

where $k = \sqrt{2\mu E}/\hbar$ and $0 \le r \le a$. Equation (9) is the so-called spherical Bessel equation which has the solutions $j_l(kr)$ and $n_l(kr)$, where $j_l(kr)$ is the spherical Bessel

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Table 1: The zeros β_{ln} of the spherical Bessel function of order l, for a few values of l and n.

β_{ln}	$n=1$	$n=2$	$n=3$	$n=4$
$l=0$	π	2π	3π	4π
$l=1$	4.49341	7.72525	10.9041	14.0662
$l=2$	5.76346	9.09501	12.3229	15.5146
$l=3$	6.98793	10.4171	13.6980	16.9236
$l=4$	8.18256	11.7049	15.0397	18.3013
$l=5$	9.35581	12.9665	16.3547	19.6532

Table 2: Eigen-energies E_{ln}, in units of $\pi^2\hbar^2/2\mu a^2$, for a few values of l and n.

E_{ln}	$n=1$	$n=2$	$n=3$	$n=4$
$l=0$	1	4	9	16
$l=1$	2.04575	6.04680	12.0471	20.0472
$l=2$	3.36563	8.38121	15.3861	24.3883
$l=3$	4.94763	10.9950	19.0115	29.0193
$l=4$	6.78389	13.8815	22.9180	33.9361
$l=5$	8.86877	17.0352	27.1010	39.1349

function of order l and $n_l(kr)$ is the spherical Neumann function of order l [4].

The spherical Neumann functions $n_l(kr)$ are discarded, since they are divergent at the center of the spherical well $r = 0$ [$n_l(r) \approx r^{-(l+1)}$ for $r \ll 1$] [1–3]. By applying the conventional boundary condition at $r = a$, *i.e.*, $R(a) = 0$, the allowed values of k are the roots of the equation $j_l(ka) = 0$. Let β_{ln} be the n-th zero of the spherical Bessel function of order l. Thus, $k_{ln} = \beta_{ln}/a$, and the eigen-energies are $E_{ln} = \hbar^2\beta_{ln}^2/2\mu a^2$. Few zeros β_{ln} of the spherical Bessel function of order l are presented in table 1. Also, few eigen-energies E_{ln}, in units of $\pi^2\hbar^2/2\mu a^2$, are presented in table 2.

Corresponding to each eigen-energy E_{ln}, the eigenstates are

$$\psi^m_{l\,n}(r,\theta,\phi) = R_{ln}(r)Y^m_l(\theta,\phi) = A_{ln}j_l(\beta_{ln}\, r/a)Y^m_l(\theta,\phi), \tag{10}$$

where A_{ln} is a normalization constant. Each eigenstate $\psi^m_{l\,n}$ is normalized in accordance with

$$\int |\psi^m_{ln}|^2 r^2 \sin\theta\, \mathrm{d}r\, \mathrm{d}\theta\, \mathrm{d}\phi = \int |R_{ln}|^2 r^2 \mathrm{d}r \int |Y^m_l|^2 \sin\theta\, \mathrm{d}\theta\, \mathrm{d}\phi = 1. \tag{11}$$

Because Y^m_l are orthonormal, A_{ln} is determined by

$$\int_0^a |R_{ln}|^2 r^2 \mathrm{d}r = \int_0^a |A_{ln}j_l(\beta_{ln}r/a)|^2 r^2 \mathrm{d}r = 1. \tag{12}$$

Because of $[\hat{\mathrm{H}}, \hat{\mathrm{L}}^2] = 0$, $[\hat{\mathrm{H}}, \hat{\mathrm{L}}_z] = 0$ and $[\hat{\mathrm{L}}^2, \hat{\mathrm{L}}_z] = 0$, the three operators $\hat{\mathrm{H}}$, $\hat{\mathrm{L}}^2$ and $\hat{\mathrm{L}}_z$ have common eigenstates for an eigen-energy. As a consequence of $[\hat{\mathrm{L}}^2, \hat{\mathrm{L}}_z] = 0$, each energy level E_{ln} is $(2l+1)$-fold degenerate.

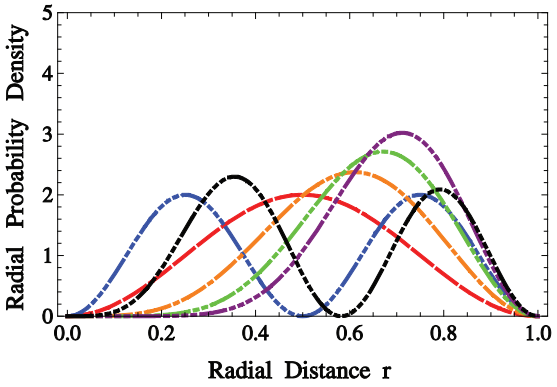

Fig. 1: (Color online) The radial probability densities of eigenstates in energy levels E_{01}, E_{11}, E_{21}, E_{02}, E_{31} and E_{12}, are shown as a dashed red line, dot-dashed orange line, two-dots-dashed green line, three-dots-dashed blue line, four-dots-dashed purple line and five-dots-dashed black line, respectively. The radial distance r is in units of a.

According to eq. (12), for an eigenstate $\psi^m_{l\,n}$, the radial probability density for finding the particle at a distance r from the center of the spherical well is $P_{ln}(r) = |R_{ln}(r)|^2 r^2$. For all eigenstates $\psi^m_{l\,n}$, their radial probability densities are zero at both the boundary $r = a$ and the center $r = 0$ of the spherical well. The radial probability densities of eigenstates in the lowest few energy levels are illustrated in fig. 1. The radial probability densities for finding the particle at the center and the boundary of the spherical well are zero.

The currently accepted solution of the infinite spherical well has been accepted without a doubt. However, it seems peculiar that the radial probability density of the particle at the center of the spherical well is zero. The usual reason to abandon the solution $n_0(kr) = -\cos(kr)/(kr)$ of eq. (9) is unconvincing. Although $n_0(kr)$ is divergent at $r = 0$, $r\, n_0(kr)$ is finite at $r = 0$, and is square-integrable. Therefore, $n_0(kr)$ is permissible from the viewpoint of physics. If $n_0(kr)$ were not abandoned, then the radial probability density for finding the particle at the center of the spherical well would not be zero.

Solve the problem by using self-adjointness of the Hamiltonian operator. – Because the particle is confined inside the spherical well, the regions outside the well are irrelevant. Therefore, the wave functions under consideration are defined inside the well only; wave functions and their derivatives are treated by the one-sided limit at the boundaries [5–9]. Owing to the self-adjointness of the Hamiltonian, boundary conditions of the system are constrained by some requirements. Substituting $R(r) = \chi(r)/r$ into eq. (6) yields

$$\hat{\mathrm{H}}_r\chi(r) = \left[-\frac{\hbar^2}{2\mu}\frac{\mathrm{d}^2}{\mathrm{d}r^2} + \frac{\hbar^2 l(l+1)}{2\mu r^2}\right]\chi(r) = E\ \chi(r). \tag{13}$$

Table 3: For $l = 0$, $\beta_{0n} = (2n-1)\pi/2$. For $l > 0$, β_{ln} are the zeros of the spherical Bessel function of order l.

β_{ln}	$n=1$	$n=2$	$n=3$	$n=4$
$l=0$	$\pi/2$	$3\pi/2$	$5\pi/2$	$7\pi/2$
$l=1$	4.49341	7.72525	10.9041	14.0662
$l=2$	5.76346	9.09501	12.3229	15.5146
$l=3$	6.98793	10.4171	13.6980	16.9236
$l=4$	8.18256	11.7049	15.0397	18.3013
$l=5$	9.35581	12.9665	16.3547	19.6532

Or

$$\frac{\mathrm{d}^2\chi(r)}{\mathrm{d}r^2} + \left(k^2 - \frac{l(l+1)}{r^2}\right)\chi(r) = 0. \tag{14}$$

As usual, the operator $\hat{\mathrm{H}}_r$ is assumed self-adjoint to determine eigenvalues. Therefore, to ensure that $\hat{\mathrm{H}}_r$ is self-adjoint, solutions $\chi(r)$ and $\chi'(r)$ of eq. (14) have to satisfy the following requirement:

$$\chi^*(r)\frac{\mathrm{d}\chi'(r)}{\mathrm{d}r} - \frac{\mathrm{d}\chi^*(r)}{\mathrm{d}r}\chi'(r)\Big|_0^a \equiv \mathcal{C}(r)\Big|_0^a = 0. \tag{15}$$

The solutions of eq. (14) are $r\ j_l(kr)$ and $r\ n_l(kr)$. Nonetheless, for $l \geq 1$, $r\ n_l(kr)$ are divergent at $r = 0$, and they are not square-integrable. Thus, the solutions $r\ n_l(kr)$ $(l \geq 1)$ are discarded from the viewpoint of physics. Consequently, the solutions needed to be considered reduce to $r\ j_l(kr)$ and $r\ n_0(kr)$. In the following, we present two cases of solutions of the problem, as an example.

Case I: Consider the solutions $r\ j_l(kr)$. By the property of Bessel function, $j_l(r) \approx r^l/(2l+1)!!$ for $r \ll 1$, for arbitrary $\chi(r) = r\ j_l(kr)$ and $\chi'(r) = r\ j_l(k'r)$, $\mathcal{C}(0) = 0$ at $r = 0$. If the solutions $\chi(r) = r\ j_l(kr)$, for any k, satisfy the boundary condition $\chi(a) = 0$ at $r = a$, then such a boundary condition fulfills the requirement given by eq. (15). The boundary condition $\chi(a) = a\ j_l(ka) = 0$ is equivalent to the conventional boundary condition $R(a) = j_l(ka) = 0$. Therefore, the eigen-energies and the eigenstates of this case are just those of the currently accepted solution as given in the first section.

Case II: Because $r\ n_0(kr)$ is physically feasible, consider the solutions: $r\ n_0(kr)$ for $l = 0$, and $r\ j_l(kr)$ for $l > 0$. For $l = 0$, $\mathcal{C}(0) = 0$ at $r = 0$, for arbitrary $\chi(r) = r\ n_0(kr) \sim \cos(kr)$ and $\chi'(r) = r\ n_0(k'r) \sim \cos(k'r)$. Also, for $l > 0$, $\mathcal{C}(0) = 0$ at $r = 0$, for arbitrary $\chi(r) = r\ j_l(kr)$ and $\chi'(r) = r\ j_l(k'r)$. The boundary condition at $r = a$, $\chi(a) = 0$, fulfills the requirement given by eq. (15).

By imposing this boundary condition at $r = a$, for $l = 0$, the allowed values of k are $k_{0n} = (2n-1)\pi/2a$, where $n = 1, 2, 3, \ldots$. Here, the first subscript 0 in k_{0n} indicates $l = 0$. Thus, the eigen-energies are $E_{0n} = \hbar^2 k_{0n}^2/2\mu a^2$. Corresponding to each eigen-energy E_{0n}, the eigenstate is

$$\psi^0_{0\,n}(r,\theta,\phi) = R_{0n}(r)Y^0_0(\theta,\phi) = A_{0n}\, n_0(k_{0n}\ r)Y^0_0(\theta,\phi), \tag{16}$$

where A_{0n} is a normalization constant. For $l > 0$, with this boundary condition, the allowed values of k are the roots of the equation $j_l(ka) = 0$. Thus, the eigenstates $\psi^m_{l\,n}$ are those of the currently accepted solution, eq. (10). Few values of β_{ln} and E_{ln} are presented in tables 3 and 4, respectively. The radial probability densities of eigenstates in the lowest few energy levels are illustrated in fig. 2. For the eigenstates ψ^0_{0n}, their radial probability densities $P_{0n}(r)$ are not zero at the center of the spherical well. Thus, the radial probability density for finding the particle at the center of the spherical well is not zero.

Table 4: Eigen-energies E_{ln} in units of $\pi^2\hbar^2/2\mu a^2$.

E_{ln}	$n=1$	$n=2$	$n=3$	$n=4$
$l=0$	1/4	9/4	25/4	49/4
$l=1$	2.04575	6.04680	12.0471	20.0472
$l=2$	3.36563	8.38121	15.3861	24.3883
$l=3$	4.94763	10.9950	19.0115	29.0193
$l=4$	6.78389	13.8815	22.9180	33.9361
$l=5$	8.86877	17.0352	27.1010	39.1349

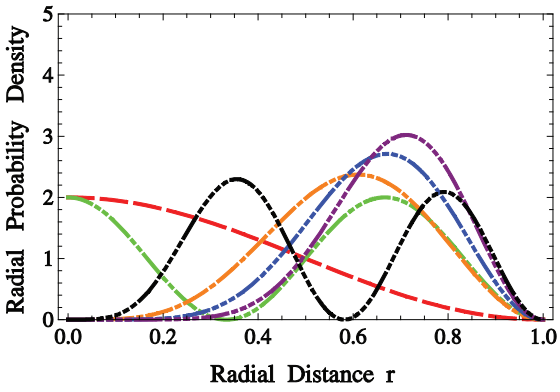

Fig. 2: (Color online) The radial probability densities of eigenstates in energy levels E_{01}, E_{11}, E_{02}, E_{21}, E_{31} and E_{12}, are shown as a dashed red line, dot-dashed orange line, two-dots-dashed green line, three-dots-dashed blue line, four-dots-dashed purple line and five-dots-dashed black line, respectively. The radial distance r is in units of a.

It should be noted that there are many more boundary conditions, other than the conventional one, satisfying the requirement given by eq. (15) [10]. Therefore, there exist many different solutions corresponding to different boundary conditions. The only solution presented in Case II is to point out an error in the currently accepted solution which is in general largely unrecognized.

Conclusion . – It seems peculiar that the radial probability density of the particle at the center of the spherical

well is zero, according to the currently accepted solution. The peculiarity is due to the abandoning of the spherical Neumann function $n_0(kr)$. The reason to abandon $n_0(kr)$ is not incontrovertible from the viewpoint of physics. Additional solutions are obtained by considering the physically feasible solution $r\ n_0(kr)$. For the additional solutions, the radial probability density of the particle at the center of the spherical well is not necessarily zero. The peculiarity of the currently accepted solution is resolved.

There is an infinity of possible boundary conditions with quite different physical characteristics [7]. Some of them will preserve time-reversibility, some parity and some energy positivity. States stationary in one solution are non-stationary in others. The energy spectra are varying in a non-linear way. As there is only a single reality, only one of these many solutions can be the correct one. To find it by sound physical arguments is a major open problem.

* * *

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