On the wave mechanics of a particle in two different impenetrable spherical cavities

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Abstract
Wave mechanics of a particle in an impenetrable spherical cavity with and without a hard core scattering potential of size $\epsilon$ ($\epsilon \to 0$) at its center is critically analyzed. It makes marginal but important modifications in our present understanding of the energy eigen values of such particles.

Key words: Quantum particle, spherical cavity.

1. Introduction
Wave mechanics of a particle, placed in widely different potentials and confinements (e.g., 1-D, 2-D and 3-D boxes, spherical cavity, etc.), has been a subject of great significance and persisting investigation for various reasons. For example, the study of a particle in a spherically symmetric potential $V(r)$ helps in understanding several physical systems such as hydrogen atom, atomic nucleus, electron bubble, quantum scattering of particles, etc. In this paper, we make a critical analysis of two separate spherical impenetrable cavities [say, Cavity-(i) and Cavity-(ii) of radii $R$ with centers identified by point “C”] with a point particle, trapped inside. Each of these cavities within its bounds has zero potential at all points except at C of Cavity-(i) which is assumed to be occupied by a hard core sphere (of radius $\epsilon \sim 0^+$, -a little more than 0) representing a $V(r)$, defined by $V(r \leq \epsilon) = \infty$ and $V(r > \epsilon) = 0$. We note that the eigen energy solutions for a particle constrained to move under the influence of a $V(r)$ are obtained by solving the radial part of its 3-D Schrödinger equation

$$\frac{1}{r^2} \frac{d}{dr} \left( r^2 \frac{dR_l(r)}{dr} \right) + \left[ \frac{2M}{\hbar^2}(E - V(r)) - \frac{l(l+1)}{r^2} \right] R_l(r) = 0. \quad (1)$$
Here, $M = \text{mass of the particle}$, $\hbar = h/2\pi$ (with $h$ being the Planck’s constant) and $R_l(r)$ (with $l$ representing orbital angular momentum of the state of the particle) is an eigen function of eigen energy $E$. Although, as defined above, Cavity-(i) and Cavity-(ii) are physically different systems for the potential they offer to the motion of the trapped particle, the known energy eigen values, $E_{n,l}(i)$ ($n$ being the principal quantum number) of the particle in Cavity-(i), obtainable from $^16$ ($\text{cf.}$, Eqn.5 and its generalization for all $l$, as concluded in Section 2.6) and $E_{n,l}(ii)$ of the particle in Cavity-(ii), available from several graduate texts $^3$-$^5$, satisfy $E_{n,l}(i) = E_{n,l}(ii)$ ($\text{cf.}$, Eqn.8 and Section 2.6). This unexpected equality motivated us to investigate its origin and to suggest correct values of $E_{n,l}(ii)$.

2. Analysis and Discussion

2.1 Unexpected Equality of $E_{n,0}(i)$ and $E_{n,0}(ii)$

Eqn.1 has been solved by Huang and Yang $^16$ for a particle trapped in the space between two concentric impenetrable spherical surfaces of radii $R$ and $a$ ($\text{with } R > a$). Using the boundary condition, $R_{l=0}(r = R) = R_{l=0}(r = a) = 0$, they obtained

$$R_0(r) = B \frac{\sin k(r - a)}{r} \text{ for } a < r < R \text{ and } R_0(r \leq a) = 0$$

(2)

where $B$ stands for normalization constant and

$$k_{n,l=0} = \frac{\pi n}{(R - a)}, \quad n = 1, 2, 3, \ldots$$

(3)

which represent the allowed values of momentum wave vector $k$. Using $a = \epsilon$, we have

$$k_{n,0} = \frac{\pi n}{R - \epsilon} = \frac{\pi n}{R}, \quad \text{as } R >> \epsilon \quad n = 1, 2, 3, \ldots,$$

(4)

and

$$E_{n,0}(i) = \frac{n^2 \hbar^2}{8MR^2}$$

(5)

and

$$R_0(r) = B \frac{\sin [k(r - \epsilon)]}{r} \approx B \frac{\sin kr}{r} \text{ at } r > \epsilon \text{ and } R_0(r \leq \epsilon) = 0$$

(6)

for the particle in Cavity-(i). However, what follows from $^3$-$^4$, we also have

$$E_{n,0}(ii) = \frac{n^2 \hbar^2}{8MR^2}$$

(7)

which can be compared with Eqn.5 to discover an equality,

$$E_{n,0}(i) = E_{n,0}(ii),$$

(8)

not expected for a particle placed in two physically different cavities. This underlines the problem that we intend to resolve in this paper.
2.2 Equivalence of Plane Wave and Spherical Waves

When the Schrödinger equation for a free particle, expressed in spherical polar coordinates, is solved one finds that different states of the particle are described by spherical waves \(^3,^4\) (centered around \(r = 0\) of the coordinate system) whose radial part is expressed by

\[ R_l(r) = A_l j_l(kr) \]  

(9)

which represents the solution of Eqn.1 with \(V(r) = 0\); here \(A_l\) are normalization constants and \(j_l(kr)\) are spherical Bessel functions. However, when we solve the Schrödinger equation expressed in Cartesian coordinates, we find that the same particle is described\(^1,^2\) by a plane wave,

\[ u_k(r) = e^{ikr} \]  

(10)

which is presumed to have unit normalization; here \(p = \hbar k\) and \(r\), respectively, represent momentum and position vector of the particle. This indicates an obvious \textit{inter-relationship} between the two descriptions of a free particle and in what follows from\(^1−^6\), we have

\[ e^{ikr} = \sum_{l=0}^{\infty} \sum_{m=-l}^{l} R_l(r) Y_{lm}(\theta, \phi), \]  

(11)

for a particle moving in any general direction (here \(Y_{lm}(\theta, \phi)\) are spherical harmonics) and

\[ e^{ikz} = \sum_{l=0}^{\infty} R_l(r) P_l(\theta) \]  

(12)

for a particle moving in \(z\)-direction (here \(P_l(\theta)\) are associated Legendre polynomials). One uses\(^3,^4\) certain boundary conditions on \(R_l(r)\) to determine \(E_{n,l}(ii)\) and, in doing so, it is implicitly assumed that spherical waves, \(R_l(r)\), originate at the center, \(C\), of Cavity-(ii) which, however, violates cause and effect relationship (\textit{cf.} Section 2.3).

2.3 Physical relevance of Eqn.11

We have no doubt that Eqn.11 (or Eqn.12) is a mathematically sound relation, but it is important to emphasize that a plane wave \([u_k(r), \text{Fig.1(a)}]\) would transform into spherical waves only when it meets a scatterer \([a \text{ source of scattering potential, } V(r)]\) and this inference is corroborated by the experimental fact that neither a ray of light, nor a beam of particles, is observed to have its scattering around an arbitrary point on its path; \textit{the point should be occupied by a scatterer} as a source of \(V(r)\). To understand this, it may be noted that the transformation of a plane wave (Fig. 1(a)) into spherical waves (Fig.1(b)) physically means that the incoming particles represented by the plane wave deviate from their paths and turn to move along any of the infinite many arrows having their single cross point \((r = 0)\) \([\text{cf.}, \text{Figs.1(c)}]\) which also represents the center of spherical waves \([\text{cf.}, \text{Fig.1(b)}]\). However, as a \textit{law of nature}, such a deviation is possible
only if the cross point of the arrows [Fig.1(c)] is occupied by a source of potential \( V(r) \) which can serve as the origin of a deviating force. In fact, it is for this reason that the partial wave theory of scattering of a beam of particles uses Eqn.12 to convert an incoming plane wave into spherical waves only around the location of a scatterer (and not around any arbitrary point) and succeeds reasonably well in accounting for the experimentally observed scattering cross sections\(^1\text{--}^6\) and other aspects.

In this context, it may be noted that if a single particle happens to repeatedly meet a \( V(r) \) (for its physical situations such as confinement in a spherical cavity) and get scattered in different directions [say along infinitely many possible lines passing through the center \( r = 0 \) of \( V(r) \)], it would also render an overall result which could be expressed in terms of spherical waves. This explains how a state of a single particle (trapped in a spherical cavity), which at any instant has a linear motion before and after an event of collision with a scatterer [be it on the surface or on at \( C \), in case of Cavity-(i)], can be identified with spherical waves, originating from the scatterer, when one sees collective result of infinite many collisions with the scatterer. This account is consistent with our understanding of the interference pattern obtained from a double slit interferometer in which only one electron is allowed to pass through its slits at a given time but the experiment is performed by using very large number of monoenergetic electrons\(^17\). While, each electron hitting the viewer’s screen leaves its record only at one point, the interference pattern emerges as a culmination of a very large number of points where different electrons hit the screen one by one\(^17\).

A hard sphere of radius \( \epsilon \) [i.e. a \( V(r) \)], presumed to occupy \( C \) of Cavity-(i), renders a clear cause for the scattering of the trapped particle and hence, for the transformation of a plane wave into spherical waves at this point. Evidently, the spherical waves (representing the scattering of particle) so produced, have to have their center at the said \( C \) point; in other words \( r = 0 \) of \( R_l(r) \) of these waves is located at the \( C \) of Cavity-(i). However, the particle in Cavity-(ii) has no reason to get scattered around its \( C \), because it finds no source of scattering potential at this point. Naturally, the implicit assumption (behind \( E_{n,l(ii)} \), - reported in\(^3,\)\(^4\)) that a plane wave representing the trapped particle can burst into spherical waves at the \( C \) of Cavity-(ii), is incorrect. In what follows from these observations, the center \( r = 0 \) of spherical waves (\( R_l(r) \)), representing the scattering of particles, falls only at the \( r = 0 \) of scattering potential \( V(r) \) and this represents an important aspect for the transformation of a plane wave into spherical waves in the domain of physics.

2.4 Meaning of \( R_l(r) \) and \( \chi_l(r) \)

We note that Eqn.1 can be transformed into

\[
\frac{d^2\chi_l(r)}{dr^2} + \left[ \frac{2M}{\hbar^2}(E - V(r)) - \frac{l(l + 1)}{r^2} \right] \chi_l(r) = 0, \tag{13}
\]
by using

\[ R_l(r) = \frac{\chi_l(r)}{r}. \]  

(14)

While, this means that solutions of Eqn.1 can be obtained by solving Eqn.13 for its eigen energy \( E \) and corresponding \( \chi_l(r) \), it also helps in finding the meaning of \( R_l(r) \) in relation to that of \( \chi_l(r) \). \( \chi_l(r) \) represents radial probability of the particle along a line passing through the scatterer, where as, \( R_l(r) \) (radial part of the spherical wave) represents the distribution of the said linear probability (\textit{with equal probability}) over other identical lines (\textit{infinitely large in number}). This can be clarified by using \( |R_l(r)| = |\chi_l(r)|/\sqrt{4\pi r} \), a slightly modified form of Eqn.14 which renders

\[ |R_l(r)|^2 = \frac{|\chi_l(r)|^2}{4\pi r^2}. \]  

(15)

Since, the said modification involves only a constant factor, \( 1/\sqrt{4\pi} \), Eqn.15 is consistent with Eqn.13. It may, therefore, be concluded that while, \( \chi_l(r) \) represents the amplitude of the radial probability of finding the particle at a point on a radial line at a distance \( r \) from the scatterer, \( R_l(r) \) represents the amplitude of the uniform distribution of the probability \( |\chi_l(r)|^2 \) over all points on \( 4\pi r^2 \) surface area of the shell of radius \( r \) around the scatterer. In other words \( r \) appearing in the denominator of Eqn.14 signifies only this distribution and \( \chi_l(r) \) carries full information about the physical state the particle and allowed energy values. Evidently, it is sufficient to put the one dimensional boundary condition on \( \chi_l(r) \), the representation of the radial distribution along a line.

2.5 Nature of Waves in Cavity-(i) and Cavity-(ii)

The hard core potential in Cavity-(i) scatters the particle around its C and produces spherical waves centered at this point. These waves can be seen to have two parts of their journey: (Part-1) originating from C, they move away to strike on the cavity surface, and (Part-2) reflected back from the said surface, they converge at C from where they turn back to repeat the cycle of Part-1 and Part-2. However, as cavity-(ii) offers no scattering potential to the trapped particle at its center C, spherical waves are not expected to originate from this point. To believe that the particle in Cavity-(ii) assumes a state represented by spherical waves, we use the fact that the surfaces of Cavity-(ii) and Cavity-(i) offer a potential of \textit{identical form} to scatter/reflect the particle. Naturally, spherical waves for the particle in Cavity-(ii) can originate from its surface, in a manner such waves (Part-2) are assumed to originate from the surface of Cavity-(i); to understand the said manner, it may be noted that a particle colliding at any point on the surface is likely to get scattered along any of the infinite many arrows passing through this point. Since all points on the inner surface are identical, the particle gets identically scattered from them and the net effect is a spherical wave front [Fig. 1(d) shows how it could be constructed from the spherical wavelets emerging from all such points] which moves towards the C of the cavity. While in Cavity-(i) this wave front is scattered back to move toward the
cavity surface, it is natural this wave front in Cavity-(ii) crosses the center C without getting scattered from it [in contrast to their obvious scattering from the C of Cavity-(i)] and it is diverted back only after its touch with the cavity surface. It is clear that the wave function, representing any state of the particle in Cavity-(ii), is not forced to vanish at its center C as it happens for the state of the particle in Cavity-(i). This, naturally, means that \( r = 0 \) of \( R_l(r) \) of these waves in Cavity-(ii) lies at its surface (where there are, indeed, scattering potentials) not at its C.

2.6 Eigen Values of the Particle in Cavity-(i) and Cavity-(ii)

Now, having a clear qualitative picture of the nature of the waves in these two cavities, let us calculate the energy eigen values. Considering that each point on the spherical wall of these cavities is a center \((r = 0)\) of strongly repulsive potential \( V(r) \), we find that on any radial line in Cavity-(i), scattering potentials are present with their centers at three points, (see three dark spherical dots marked as 1, 2, and 3 in Fig. 1(e)), while, in Cavity-(ii) they are present only at two points (see two dark spherical dots marked as 1 and 2 in Fig. 1(f)). It is common to observe a single system having several centers of scattering potential(s), for example, numerous constituents (atoms/molecules) of a solid serve as centers the scattering of x-ray photons, electrons, neutrons, etc.

In what follows from Section 2.3, the origin of spherical waves is synonym with the center \( r = 0 \) of \( V(r) \), and Section 2.4, \( \chi_l(r) \), subjected to appropriate boundary conditions, is sufficient to determine the energy eigen values of the particle. Guided by these observations, we choose the origin \( r = 0 \) of \( \chi_l(r) \) only at any of the three points for Cavity-(i) [viz. points 1, 2 and 3 in Fig.1(e)] and any of the two points for Cavity-(ii) [viz. points 1 and 2 in Fig. 1(f)] from where the scattering of the particle can take place. In this context, as concluded above, \( R_l(r) \) has zero value at the location \( r = 0 \) (even for \( l = 0 \) (cf. Eqn.6) which implies that \( \chi_l(r) \) is also zero at this location. For an identical choice for both cavities, we prefer to choose point 1 (or 2) [Figs.1(e) and 1(f)] as the center of \( V(r) \) and the origin of \( \chi_l(r) \) and use the location of nearest scattering center on the radial line as a point where \( \chi_l(r) \) has to have its node (zero value); however, for Cavity-(i), one may also choose point 3 as the origin \( r = 0 \) of \( \chi_l(r) \) and point 1 (or 2) as a location where it has to have a node. Evidently, the nodes of \( \chi_l(r) \) are separated at the maximum by \( R \) in case of Cavity-(i) and by \( D(= 2R) \) in case of Cavity-(ii).

Since, \( \chi_l(r) = rR_l(r) = rA_lj_l(kr) \) and \( j_l(kr) \) has many zeroes at \( kr = \beta_{n,l}\pi \) (where \( \beta_{n,l} \) is a number as defined in\(^3\)), the energy eigen values for the particle in Cavity-(i) are given by

\[
E_{n,l}(i) = \frac{\beta_{n,l}^2 \hbar^2}{8MR^2}
\]  

by setting

\[
k_{n,l}R = \beta_{n,l}\pi, \tag{17}\]
and those in Cavity-(ii) are given by

\[ E_{n,l}^{(ii)} = \frac{\beta_{n,l}^2 h^2}{8MD^2} \]  \hspace{1cm} (18)

by setting

\[ k_{n,l}D = \beta_{n,l}\pi. \]  \hspace{1cm} (19)

We now note that our \( E_{n,l}^{(i)} \) (Eqn.16) not only encompasses Eqn.5, but also generalizes Eqn.8 for all values of \( l \) as it is equal to \( E_{n,l}^{(ii)} = \beta_{n,l}^2 h^2/8MR^2 \) concluded in\(^3,4\). However, \( E_{n,l}^{(ii)} \) (Eqn.18), concluded from this study, differs from \( E_{n,l}^{(ii)} \) of\(^3,4\) by a factor of 1/4. It is because, the steps of finding \( E_{n,l}^{(ii)} \) in\(^3,4\) somehow presume that \( u_k(r) \) of the particle bursts into spherical waves at C of Cavity-(ii), although necessary \( V(r) \) does not exist there (as discussed in section 2.3); this explains why \( E_{n,l}^{(ii)} \), reported in\(^3,4\), exactly matches with our \( E_{n,l}^{(i)} \) (Eqn.16) for Cavity-(i) which, indeed, has an infinitely small hard core scattering potential at its center. Since, the present analysis does not make the said presumption, it renders \( E_{n,l}^{(ii)} \) (Eqn.18) which differs from \( E_{n,l}^{(i)} \) (Eqn.16), as expected.

3. Conclusion

As discussed in section 2.3, we find that the use of Eqn.11 (or, Eqn.12) in obtaining \( E_{n,l}^{(ii)} = \beta_{n,l}^2 h^2/8MR^2 \) (as concluded in\(^3,4\)) is not proper. Further, it is for this reason, that one finds an unrealistic equality between \( E(i) \) and \( E(ii) \) (cf., Eqn.8). Guided by this fact, we analysed the problem more critically and discovered that \( E_{n,l}^{(ii)} \) (Eqn.18) is clearly different from \( E_{n,l}^{(i)} \) (Eqn.16) by a factor of 1/4. We hope that this would greatly help in having a better understanding of the quantum states of a particle trapped in Cavity-(i) and Cavity-(ii).

Acknowledgment: Authors are thankful to Dr. Simanta Chutia and Jeeban P. Gewali for useful interaction. The work is supported partially by DST project.
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Figure 1: Depiction of: (a) $u_k(r)$, (b) spherical waves representing scattered waves from $V(r)$ centered around $r = 0$, (c) some of the possible directions of the motion of a particle after its scattering form $V(r)$ centered around $r = 0$, (d) spherical wave front (dotted circles) constructed from scattered wavelets (represented by bunches of arrows emerging from different points on the surface) from different points on the surface, (e) one of the infinite many radial lines of Cavity-(i) and three centers (dark spherical dots) of the scattering potentials present on it and (f) one of the infinite many radial lines of Cavity-(ii) and two centers (dark spherical dots) of the scattering potentials present on it.