# Quantum mechanical derivation of the Wallis formula for Pi

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## 1 Introduction

In 2015 two physicists, Tamar Friedmann and C R Hagen produced a quantum mechanical derivation of Wallis' formula for Pi based on the hydrogen atom [1] . Some reactions to this derivation sought to divine an almost mystical link between quantum mechanics and Pi. Subsequently, Ignacio Cortese and J Antonio Garcia showed that the hydrogen atom Hamiltonian is not necessary to obtain the Wallis formula [2]. In essence, Friedmann and Hagen applied the variational method to the ground state of the hydrogen atom with the angular momentum becoming large in the classical limit of $l \to \infty$. They used a convenient trial function for their calculations and out of the calculations "popped" the Gamma function which figured essentially in obtaining Wallis' formula:

$$\frac{\pi}{2} = \frac{2 \cdot 2}{1 \cdot 3}\,\frac{4 \cdot 4}{3 \cdot 5}\,\frac{6 \cdot 6}{5 \cdot 7} \cdots \tag{1}$$

The purpose of this article is to give a detailed verification of each step in the calculations which involve essentially undergraduate level quantum mechanics, but with many calculational pitfalls. Indeed, as will be seen below, because the trial function involves spherical harmonic functions there is quite a bit of assumed knowledge in the manipulation of them and the details of that are also provided. While paper [1] is short, the fundamental calculation of the expectation of the Hamiltonian is done in one step and would no doubt have been set as a homework problem for the authors' students. You can, of course, put the integrals into Mathematica and perform the verification that way but the hand method is character building! The only other difficult part of the paper is the following limit:

$$\lim_{l\to\infty} \frac{(l+1)^2}{l+\frac{3}{2}} \Big[\frac{\Gamma(l+1)}{\Gamma(l+\frac{3}{2}}\Big]^2 = 1$$

The authors suspiciously quote some values in a footnote which suggest the convergence to 1. My guess is they used Mathematica or Matlab but there is an asymptotic expression for the ratio of two Gamma functions which allows one to show rigorously that the limit is indeed 1.

## 2 The derivation

The Schrodinger wave equation for the hydrogen atom is given by:

$$H\Psi = \Big(-\frac{\hbar^2}{2m}\nabla^2 - \frac{e^2}{r}\Big)\Psi = E\Psi \tag{2}$$

The corresponding radial equation obtained by separation of variables is (see [3], pages 779-782 for more detail ):

$$H(r)R(r) = \Big[-\frac{\hbar^2}{2m}\Big(\frac{d^2}{dr^2} + \frac{2}{r}\frac{d}{dr} - \frac{l(l+1)}{r^2}\Big) - \frac{e^2}{r}\Big]\, R(r) = ER(r) \tag{3}$$

The authors use a trial wave function of the following form:

$$\Psi_{\alpha lm} = r^l e^{-\alpha r^2} Y_l^m(\theta,\phi) \tag{4}$$

where $\alpha > 0$ is a real parameter and $Y_l^m(\theta,\phi)$ are the usual spherical harmonics. The expectation value of the Hamiltonian is given by:

$$\begin{aligned}\langle H\rangle_{\alpha l} =& \frac{\langle\Psi_{\alpha lm}|H(r)|\Psi_{\alpha lm}\rangle}{\langle\Psi_{\alpha lm}|\Psi_{\alpha lm}\rangle}\\ =& \frac{\hbar^2}{2m}\Big(l+\frac{3}{2}\Big)2\alpha - e^2\frac{\Gamma(l+1)}{\Gamma(l+\frac{3}{2})}\sqrt{2\alpha}\end{aligned} \tag{5}$$

There is quite a lot of calculation behind the jump from the first line of equation (5) to the second line as will be seen ! For those "in the zone" with the underlying theory the calculations are straightforward but require care.

The denominator in the expectation value of the Hamiltonian is $\langle\Psi_{\alpha lm}|\Psi_{\alpha lm}\rangle$ and working this integral out contains the components for the more complicated numerator.

We start first with a definition:

$$\langle\Psi_{\alpha lm}|\Psi_{\alpha lm}\rangle = \int_{\mathcal{V}} \Psi^*_{\alpha lm}\,\Psi_{\alpha lm}\,d\mathcal{V} \tag{6}$$

The volume $\mathcal{V}$ is three space and since spherical harmonics are used our differential volume will be:

$$d\mathcal{V} = r^2\sin\theta\,d\theta\,d\phi\,dr \tag{7}$$

We first need to give the form of the spherical harmonic component of (4):

$$Y_l^m(\theta,\phi) = (-1)^m\sqrt{\frac{(2l+1)(l-m)!}{4\pi(l+m)!}}P_l^m(\cos\theta)e^{im\phi} \tag{8}$$

Equation (8) holds for $l = 0, 1, 2, 3, \dots$ and $m = -l, -l+1, \dots, l-1, l$ (see [3] pages 678-689).

Note that the $P_l^m(x)$ are associated Legendre polynomials which satisfy the following:

$$P_l^m(x) = (1-x^2)^{\frac{m}{2}} \frac{d^m}{dx^m} P_l(x) \tag{9}$$

The following is the orthogonality property:

$$\int_0^\pi P_k^m(\cos\theta)\, P_l^m(\cos\theta)\, \sin\theta\, d\theta = \frac{2(l+m)!}{(2l+1)(l-m)!}\, \delta_{kl} \tag{10}$$

$\delta_{kl}$ is the Kronecker delta ie $\delta_{kl} = 1$ when $k = l$ and 0 when $k \neq l$.

The properties of Legendre polynomials $P_l(x)$ can be found in many textbooks eg Chapter 9 of [4]. A proof of (10) is in the Appendix.

Writing out (6) in detail we get:

$$\begin{aligned}
\langle \Psi_{\alpha l m} | \Psi_{\alpha l m} \rangle &= \int_0^{2\pi} \int_0^\infty \int_0^\pi r^l e^{-\alpha r^2} Y_l^{*\,m}(\theta,\phi) r^l e^{-\alpha r^2} Y_l^m(\theta,\phi)\, r^2 \sin\theta\, d\theta\, dr\, d\phi \\
&= \int_0^{2\pi} \int_0^\infty \int_0^\pi r^{2l} e^{-2\alpha r^2} \frac{(2l+1)(l-m)!}{4\pi(l+m)!} [P_l^m(\cos\theta)]^2\, r^2 \sin\theta\, d\theta\, dr\, d\phi \\
&= 2\pi\, \frac{(2l+1)(l-m)!}{4\pi(l+m)!} \int_0^\infty r^{2l+2} e^{-2\alpha r^2}\, dr \int_0^\pi [P_l^m(\cos\theta)]^2\, \sin\theta\, d\theta \\
&= 2\pi\, \frac{(2l+1)(l-m)!}{4\pi(l+m)!} \int_0^\infty r^{2l+2} e^{-2\alpha r^2}\, dr \,\times\, \frac{2(l+m)!}{(2l+1)(l-m)!} \\
&= \int_0^\infty r^{2l+1} e^{-2\alpha r^2}\, r\, dr \\
&= \int_0^\infty \left(\frac{y}{2\alpha}\right)^{l+\frac{1}{2}} e^{-y}\, \frac{dy}{4\alpha} \\
&= \frac{1}{2(2\alpha)^{l+\frac{3}{2}}} \int_0^\infty \left(\frac{y}{2\alpha}\right)^{l+\frac{3}{2}-1} e^{-y}\, dy \\
&= \frac{1}{2(2\alpha)^{l+\frac{3}{2}}} \Gamma(l+\frac{3}{2})
\end{aligned} \tag{11}$$

Note that in integrating $\int_0^\infty r^{2l+1} e^{-2\alpha r^2}\, r\, dr$ the substitution $y = 2\alpha r^2$ so that $dy = 4\alpha r dr$. Recall that $\Gamma(l) = \int_0^\infty x^{l-1} e^{-x}\, dx$ , $z\Gamma(z) = \Gamma(z+1)$, $l! = \Gamma(l+1)$ and $\Gamma(\frac{1}{2}) = \sqrt{\pi}$.

We now have the building blocks for the numerator. As can be seen, we only have to integrate the radial part of the function since the angular components of the integral normalise to 1.

Writing the numerator of (5) out we have, after noting that the angular parts can be pushed through the Hamiltonian and cancel to 1 as in (11), we have:

$$\begin{aligned}
\langle\Psi_{\alpha lm}|H(r)|\Psi_{\alpha lm}\rangle =& \int_0^\infty r^l e^{-\alpha r^2}\Big[-\frac{\hbar^2}{2m}\Big(\frac{d^2}{dr^2}+\frac{2}{r}\frac{d}{dr}-\frac{l(l+1)}{r^2}\Big)-\frac{e^2}{r}\Big]\underbrace{(r^l e^{-\alpha r^2})}_{\text{The operator only acts on this}}\, r^2\,dr\\
=& \int_0^\infty r^l e^{-\alpha r^2}\Big[-\frac{\hbar^2}{2m}\Big(\frac{d^2}{dr^2}(r^l e^{-\alpha r^2})\Big)+\frac{2}{r}\frac{d}{dr}(r^l e^{-\alpha r^2})-\frac{l(l+1)}{r^2}(r^l e^{-\alpha r^2})\Big)\\
&-\frac{e^2}{r}(r^l e^{-\alpha r^2})\Big]r^2\,dr\\
=& \int_0^\infty r^l e^{-\alpha r^2}\Big[-\frac{\hbar^2}{2m}\Big(\frac{d^2}{dr^2}(r^l e^{-\alpha r^2})\Big)\Big]r^2\,dr+\int_0^\infty r^l e^{-\alpha r^2}\Big[-\frac{\hbar^2}{2m}\frac{2}{r}\frac{d}{dr}(r^l e^{-\alpha r^2})\Big]r^2\,dr\\
&+\int_0^\infty r^l e^{-\alpha r^2}\Big[\frac{\hbar^2}{2m}\Big(\frac{l(l+1)}{r^2}(r^{l+2}e^{-\alpha r^2})\Big)\Big]dr-\int_0^\infty\frac{e^2}{r}(r^{2l+2}e^{-2\alpha r^2})\,dr
\end{aligned}\tag{12}$$

We now deal with each of the four integrals in (12) separately.

$$\begin{aligned}
-\int_0^\infty\frac{e^2}{r}(r^{2l+2}e^{-2\alpha r^2})\,dr =& -e^2\int_0^\infty r^{2l}e^{-2\alpha r^2}r\,dr\\
=& -e^2\int_0^\infty\Big(\frac{y}{2\alpha}\Big)^l e^{-y}\frac{dy}{4\alpha}\\
=& -\frac{e^2}{2(2\alpha)^{l+1}}\int_0^\infty y^{l+1-1}e^{-y}\,dy\\
=& -\frac{e^2}{2(2\alpha)^{l+1}}\Gamma(l+1)
\end{aligned}\tag{13}$$

We now normalise (13) by (11):

$$\frac{-\frac{e^2}{2(2\alpha)^{l+1}}\Gamma(l+1)}{\frac{1}{2(2\alpha)^{l+\frac{3}{2}}}\Gamma(l+\frac{3}{2})} = -e^2\frac{\Gamma(l+1)}{\Gamma(l+\frac{3}{2})}\sqrt{2\alpha}\tag{14}$$

The next integral is:

$$\begin{aligned}
\int_0^\infty r^l e^{-\alpha r^2}\Big[\frac{\hbar^2}{2m}\Big(\frac{l(l+1)}{r^2}(r^{l+2}e^{-\alpha r^2})\Big)\Big]dr =& \frac{\hbar^2 l(l+1)}{2m}\int_0^\infty r^{2l-1}e^{-2\alpha r^2}\,r dr\\
=& \frac{\hbar^2 l(l+1)}{2m}\int_0^\infty\Big(\frac{y}{2\alpha}\Big)^{l-\frac{1}{2}}e^{-y}\frac{dy}{4\alpha}\\
=& \frac{\hbar^2 l(l+1)}{2m}\frac{1}{2(2\alpha)^{l+\frac{1}{2}}}\int_0^\infty y^{l-\frac{1}{2}}e^{-y}\,dy\\
=& \frac{\hbar^2 l(l+1)}{4m}\frac{1}{(2\alpha)^{l+\frac{1}{2}}}\int_0^\infty y^{l+\frac{1}{2}-1}e^{-y}\,dy\\
=& \frac{\hbar^2 l(l+1)}{4m}\frac{1}{(2\alpha)^{l+\frac{1}{2}}}\Gamma(l+\frac{1}{2})
\end{aligned}\tag{15}$$

We now normalise (15) by (11):

$$\begin{aligned}\frac{\frac{\hbar^2 l(l+1)}{4m}\frac{1}{(2\alpha)^{l+\frac{1}{2}}}\Gamma(l+\frac{1}{2})}{\frac{1}{2(2\alpha)^{l+\frac{3}{2}}}\Gamma(l+\frac{3}{2})} &= \frac{\hbar^2 l(l+1)}{2m}\frac{\Gamma(l+\frac{1}{2})}{\Gamma(l+\frac{3}{2})}2\alpha \\ &= \frac{\hbar^2 l(l+1)}{2m}\frac{\Gamma(l+\frac{1}{2})}{(l+\frac{1}{2})\Gamma(l+\frac{1}{2})}2\alpha \\ &= \frac{\hbar^2 l(l+1)}{2m}\frac{4\alpha}{(2l+1)}\end{aligned} \tag{16}$$

For the remaining two integrals we need the following derivatives:

$$\frac{d}{dr}\big(r^l e^{-\alpha r^2}\big) = \big(l r^{l-1} - 2\alpha r^{l+1}\big)e^{-\alpha r^2} \tag{17}$$

$$\begin{aligned}\frac{d^2}{dr^2}\big(r^l e^{-\alpha r^2}\big) &= \frac{d}{dr}\Big(l r^{l-1} - 2\alpha r^{l+1}\big)e^{-\alpha r^2}\Big) \\ &= \Big(l(l-1)r^{l-2} - 2\alpha(2l+1)r^l + 4\alpha^2 r^{l+2}\Big)e^{-\alpha r^2}\end{aligned} \tag{18}$$

The next integral is (using (17) ):

$$\begin{aligned}\int_0^\infty r^l e^{-\alpha r^2}\Big[-\frac{\hbar^2}{2m}\frac{2}{r}\frac{d}{dr}(r^l e^{-\alpha r^2})\Big]\, r^2\, dr &= \int_0^\infty r^l e^{-\alpha r^2}\Big[-\frac{\hbar^2}{2m}\frac{2}{r}\frac{d}{dr}(r^l e^{-\alpha r^2})\Big]\, r^2\, dr \\ &= \int_0^\infty r^l e^{-\alpha r^2}\Big[-\frac{\hbar^2}{2m}\frac{2}{r}\big(l r^{l-1} - 2\alpha r^{l+1}\big)e^{-\alpha r^2}\Big]\, r^2\, dr \\ &= -\frac{\hbar^2}{2m}\int_0^\infty \Big[2l r^{2l-1} - 4\alpha r^{2l+1}\Big]e^{-2\alpha r^2}\, r\, dr \\ &= -\frac{\hbar^2}{2m}\Big[2l\int_0^\infty \Big(\frac{y}{2\alpha}\Big)^{l-\frac{1}{2}} e^{-y}\frac{dy}{4\alpha} - 4\alpha\int_0^\infty \Big(\frac{y}{2\alpha}\Big)^{l+\frac{1}{2}} e^{-y}\frac{dy}{4\alpha}\Big] \\ &= -\frac{\hbar^2}{2m}\Big[\frac{l}{(2\alpha)^{l+\frac{1}{2}}}\int_0^\infty y^{l+\frac{1}{2}-1}e^{-y}dy - \frac{1}{(2\alpha)^{l+\frac{1}{2}}}\int_0^\infty y^{l+\frac{3}{2}-1}e^{-y}\, dy\Big] \\ &= -\frac{\hbar^2}{2m}\frac{1}{(2\alpha)^{l+\frac{1}{2}}}\Big[l\,\Gamma(l+\frac{1}{2}) - \Gamma(l+\frac{3}{2})\Big] \\ &= -\frac{\hbar^2}{2m}\frac{1}{(2\alpha)^{l+\frac{1}{2}}}\Big[l\,\Gamma(l+\frac{1}{2}) - (l+\frac{1}{2})\,\Gamma(l+\frac{1}{2})\Big] \\ &= \frac{\hbar^2}{4m}\frac{\Gamma(l+\frac{1}{2})}{(2\alpha)^{l+\frac{1}{2}}}\end{aligned} \tag{19}$$

As before, we normalise by (11):

$$
\begin{aligned}
\frac{\frac{\hbar^2}{4m}\frac{\Gamma(l+\frac{1}{2})}{(2\alpha)^{l+\frac{1}{2}}}}{\frac{1}{2(2\alpha)^{l+\frac{3}{2}}}\Gamma(l+\frac{3}{2})} =& \frac{\hbar^2}{4m}4\alpha\frac{1}{l+\frac{1}{2}} \\
=& \frac{\hbar^2 4\alpha}{2m}\frac{1}{2l+1}
\end{aligned}
\tag{20}
$$

The final integral is as follows (using (18) ):

$$
\begin{aligned}
\int_0^\infty r^l e^{-\alpha r^2}\Big[-\frac{\hbar^2}{2m}\Big(\frac{d^2}{dr^2}(r^l e^{-\alpha r^2})\Big)\Big]\, r^2\, dr =& \int_0^\infty r^l e^{-\alpha r^2}\Big[-\frac{\hbar^2}{2m}\Big(l(l-1)r^{l-2} - 2\alpha(2l+1)r^l + 4\alpha^2 r^{l+2}\Big)e^{-\alpha r^2}\Big]\, r^2\, dr \\
=& -\frac{\hbar^2}{2m}\int_0^\infty \Big(l(l-1)r^{2l-1} - 2\alpha(2l+1)r^{2l+1} + 4\alpha^2 r^{2l+3}\Big)\, e^{-2\alpha r^2}\, r\, dr \\
=& -\frac{\hbar^2}{2m}\int_0^\infty \Big[l(l-1)\Big(\frac{y}{2\alpha}\Big)^{l-\frac{1}{2}} e^{-y} - 2\alpha(2l+1)\Big(\frac{y}{2\alpha}\Big)^{l+\frac{1}{2}} e^{-y} \\
& + 4\alpha^2\Big(\frac{y}{2\alpha}\Big)^{l+\frac{3}{2}} e^{-y}\Big]\frac{dy}{4\alpha} \\
=& -\frac{\hbar^2}{2m}\int_0^\infty \Big[\frac{l(l-1)}{2(2\alpha)^{l+\frac{1}{2}}} y^{l+\frac{1}{2}-1} e^{-y} - \frac{(2l+1)}{2(2\alpha)^{l+\frac{1}{2}}} y^{l+\frac{3}{2}-1} e^{-y} \\
& + \frac{\alpha}{(2\alpha)^{l+\frac{3}{2}}} y^{l+\frac{5}{2}-1} e^{-y}\Big] dy \\
=& -\frac{\hbar^2}{2m}\Big[\frac{l(l-1)}{2(2\alpha)^{l+\frac{1}{2}}}\Gamma(l+\frac{1}{2}) - \frac{(2l+1)}{2(2\alpha)^{l+\frac{1}{2}}}\Gamma(l+\frac{3}{2}) + \frac{\alpha}{(2\alpha)^{l+\frac{3}{2}}}\Gamma(l+\frac{5}{2})\Big] \\
=& -\frac{\hbar^2}{2m}\Big[\frac{l(l-1)}{2(2\alpha)^{l+\frac{1}{2}}}\Gamma(l+\frac{1}{2}) - \frac{(2l+1)}{2(2\alpha)^{l+\frac{1}{2}}}\Gamma(l+\frac{3}{2}) + \frac{\alpha(l+\frac{3}{2})}{(2\alpha)^{l+\frac{3}{2}}}\Gamma(l+\frac{3}{2})\Big]
\end{aligned}
\tag{21}
$$

Finally we normalise by (11):

$$
\begin{aligned}
\frac{-\frac{\hbar^2}{2m}\left[\frac{l(l-1)}{2(2\alpha)^{l+\frac{1}{2}}}\Gamma(l+\frac{1}{2})-\frac{(2l+1)}{2(2\alpha)^{l+\frac{1}{2}}}\Gamma(l+\frac{3}{2})+\frac{\alpha(l+\frac{3}{2})}{(2\alpha)^{l+\frac{3}{2}}}\Gamma(l+\frac{3}{2})\right]}{\frac{1}{2(2\alpha)^{l+\frac{3}{2}}}\Gamma(l+\frac{3}{2})} =& -\frac{\hbar^2}{2m}\Big[\frac{l(l-1)}{2(2\alpha)^{l+\frac{1}{2}}}\Gamma(l+\frac{1}{2})\frac{2(2\alpha)^{l+\frac{3}{2}}}{\Gamma(l+\frac{3}{2})} \\
& -\frac{(2l+1)}{2(2\alpha)^{l+\frac{1}{2}}}\Gamma(l+\frac{3}{2})\frac{2(2\alpha)^{l+\frac{3}{2}}}{\Gamma(l+\frac{3}{2})} \\
& +\frac{\alpha(l+\frac{3}{2})}{(2\alpha)^{l+\frac{3}{2}}}\Gamma(l+\frac{3}{2})\frac{2(2\alpha)^{l+\frac{3}{2}}}{\Gamma(l+\frac{3}{2})}\Big] \\
=& -\frac{\hbar^2}{2m}\Big[\frac{l(l-1)2\alpha}{(l+\frac{1}{2})}-(2l+1)2\alpha+2\alpha(l+\frac{3}{2})\Big] \\
=& -\frac{\hbar^2}{2m}\Big[\frac{l(l-1)4\alpha-(2l+1)^2 2\alpha+\alpha(2l+3)(2l+1)}{2l+1}\Big] \\
= -\frac{\hbar^2}{2m}\Big[\frac{4\alpha l^2-4\alpha l-8\alpha l^2-8\alpha l-2\alpha+4\alpha l^2+8\alpha l+3\alpha}{2l+1}\Big]& \\
=& -\frac{\hbar^2\alpha}{2m}\Big[\frac{1-4l}{2l+1}\Big]
\end{aligned} \tag{22}
$$

We now add (14), (16), (20) and (22) to get the final value for (5) :

$$
\begin{aligned}
-e^2\frac{\Gamma(l+1)}{\Gamma(l+\frac{3}{2})}\sqrt{2\alpha}+\frac{\hbar^2 l(l+1)}{2m}\frac{4\alpha}{(2l+1)}+\frac{\hbar^2 4\alpha}{2m}\frac{1}{2l+1}-\frac{\hbar^2\alpha}{2m}\Big[\frac{1-4l}{2l+1}\Big] =& -e^2\frac{\Gamma(l+1)}{\Gamma(l+\frac{3}{2})}\sqrt{2\alpha} \\
& +\frac{\hbar^2\alpha}{2m}\Big[\frac{4l(l+1)+4-(1-4l)}{2l+1}\Big] \\
=& -e^2\frac{\Gamma(l+1)}{\Gamma(l+\frac{3}{2})}\sqrt{2\alpha}+\frac{\hbar^2\alpha}{2m}\Big[\frac{4l^2+8l+3}{2l+1}\Big] \\
=& -e^2\frac{\Gamma(l+1)}{\Gamma(l+\frac{3}{2})}\sqrt{2\alpha}+\frac{\hbar^2\alpha}{2m}\Big[\frac{(2l+1)(2l+3)}{2l+1}\Big] \\
=& -e^2\frac{\Gamma(l+1)}{\Gamma(l+\frac{3}{2})}\sqrt{2\alpha}+\frac{\hbar^2\alpha}{2m}(2l+3) \\
=& -e^2\frac{\Gamma(l+1)}{\Gamma(l+\frac{3}{2})}\sqrt{2\alpha}+\frac{\hbar^2}{2m}(l+\frac{3}{2})2\alpha
\end{aligned} \tag{23}
$$

So (5) is correct. The verification of the rest of the paper now follows.

Because of the orthogonality property of the spherical harmonics the function $\Psi\alpha lm$ is orthogonal to any energy and angular momentum eigenstate that has a value for angular momentum different from $l$. Hence the minimisation of $\langle H\rangle_\alpha$ gives an upper bound for the lowest energy state for a given value of $l$. Bear in mind here that $\langle H\rangle_\alpha$ is an average which is being minimised. The details are:

$$\frac{\partial\langle H\rangle_{\alpha l}}{\partial\alpha} = \frac{\hbar^2}{m}(l+\frac{3}{2}) - e^2\frac{\Gamma(l+1)}{\Gamma(l+\frac{3}{2})}\times\frac{\sqrt{2}}{2\sqrt{\alpha}} \tag{24}$$

The minimum occurs when:

$$\sqrt{\alpha} = \frac{\sqrt{2}}{2\hbar^2}me^2\frac{\Gamma(l+1)}{\Gamma(l+\frac{3}{2})}\frac{1}{(l+\frac{3}{2})} \tag{25}$$

Note that $\frac{\partial^2\langle H\rangle_{\alpha l}}{\partial\alpha^2} > 0$. Plugging the values for $\alpha$ into (5) leads to:

$$\langle H\rangle^l_{\min} = \frac{-me^4}{2\hbar^2}\Big[\frac{\Gamma(l+1)}{\Gamma(l+\frac{3}{2})}\Big]^2\frac{1}{(1+\frac{3}{2})} \tag{26}$$

The exact result for the energy levels of hydrogen is ( see [5], page 417 ):

$$E_{n_r,l} = \frac{-me^4}{2\hbar^2}\frac{1}{(n_r+l+1)^2} \tag{27}$$

where $n_r = 0, 1, 2, \ldots$

Thus according to (27) the lowest energy state for a given $l$ occurs when $n_r = 0$:

$$E_{0,l} = \frac{-me^4}{2\hbar^2}\frac{1}{(l+1)^2} \tag{28}$$

The authors then look at the accuracy of the approximation represented by (26) and to this end they examine this ratio:

$$\frac{\langle H\rangle^l_{\min}}{E_{0,l}} = \frac{(l+1)^2}{(l+\frac{3}{2})}\Big[\frac{\Gamma(l+1)}{\Gamma(l+\frac{3}{2})}\Big]^2 \tag{29}$$

They assert that ratio in (29) approaches 1 for large $l$ and footnote that by reference to values of the ratio for $l = 0, 1, 2, 10, 100$. Physically, they argue that in the large $l$ limit the trial solution and the exact result correspond to strictly circular orbits and that the circularity of the trial solution orbits at large $l$ is a consequence of the fact that the uncertainty in $r^2$ , measured in units of mean square radius, is given by:

$$\frac{[\langle r^4\rangle_{\alpha l} - \big(\langle r^2\rangle_{\alpha l}\big)^2]^{\frac{1}{2}}}{\langle r^2\rangle_{\alpha l}} = \Big(l+\frac{3}{2}\Big)^{-\frac{1}{2}} \tag{30}$$

Clearly as $l \to \infty$ (30) approaches 0.

The verification of (30) is as follows.

$$\langle r^2\rangle_{\alpha l} = \frac{\langle\Psi_{\alpha lm}|r^2|\Psi_{\alpha lm}\rangle}{\langle\Psi_{\alpha lm}|\Psi_{\alpha lm}\rangle} = \frac{\text{TOP}}{\text{BOTTOM}} \tag{31}$$

$$
\begin{aligned}
\text{TOP} =& \int_0^\infty r^2 r^{2l} e^{-2\alpha r^2} r^2 \, dr \\
=& \int_0^\infty r^{2l+3} e^{-2\alpha r^2} r \, dr \\
=& \int_0^\infty (\frac{y}{2\alpha})^{l+\frac{3}{2}} e^{-y} \, \frac{dy}{4\alpha} \\
=& \frac{1}{2(2\alpha)^{l+\frac{5}{2}}} \int_0^\infty y^{l+\frac{5}{2}-1} e^{-y} \, dy \\
=& \frac{1}{2(2\alpha)^{l+\frac{5}{2}}} \Gamma(l+\frac{5}{2})
\end{aligned}
\tag{32}
$$

Using (11):

$$
\text{BOTTOM } = \frac{1}{2(2\alpha)^{l+\frac{3}{2}}} \Gamma(l+\frac{3}{2}) \tag{33}
$$

Hence:

$$
\langle r^2 \rangle_{\alpha l} = \frac{1}{2(2\alpha)^{l+\frac{5}{2}}} \Gamma(l+\frac{5}{2}) \times \frac{2(2\alpha)^{l+\frac{3}{2}}}{\Gamma(l+\frac{3}{2})} = \frac{l+\frac{3}{2}}{2\alpha} \tag{34}
$$

$$
\begin{aligned}
\langle r^4 \rangle_{\alpha l} =& \frac{\int_0^\infty r^4 r^{2l} e^{-2\alpha r^2} r^2 \, dr}{\langle \Psi_{\alpha l m} | \langle \Psi_{\alpha l m} \rangle} \\
=& \int_0^\infty r^{2l+5} e^{-2\alpha r^2} r \, dr \times \frac{2(2\alpha)^{l+\frac{3}{2}}}{\Gamma(l+\frac{3}{2})} \\
=& \int_0^\infty (\frac{y}{2\alpha})^{l+\frac{5}{2}} e^{-y} \, \frac{dy}{4\alpha} \times \frac{2(2\alpha)^{l+\frac{3}{2}}}{\Gamma(l+\frac{3}{2})} \\
=& \frac{1}{2(2\alpha)^{l+\frac{7}{2}}} \int_0^\infty y^{l+\frac{7}{2}-1} e^{-y} \, dy \times \frac{2(2\alpha)^{l+\frac{3}{2}}}{\Gamma(l+\frac{3}{2})} \\
=& \frac{\Gamma(l+\frac{7}{2})}{2(2\alpha)^{l+\frac{7}{2}}} \times \frac{2(2\alpha)^{l+\frac{3}{2}}}{\Gamma(l+\frac{3}{2})} \\
=& \frac{(l+\frac{5}{2})(l+\frac{3}{2})\Gamma(l+\frac{3}{2})}{4\alpha^2 \Gamma(l+\frac{3}{2})} \\
=& \frac{(l+\frac{5}{2})(l+\frac{3}{2})}{4\alpha^2}
\end{aligned}
\tag{35}
$$

Finally, plugging the relevant values into (30) we have:

$$
\begin{aligned}
\frac{[\langle r^4\rangle_{\alpha l} - \big(\langle r^2\rangle_{\alpha l}\big)^2]^{\frac{1}{2}}}{\langle r^2\rangle_{\alpha l}} =& \frac{\Big[\frac{(l+\frac{5}{2})(l+\frac{3}{2})}{4\alpha^2} - \frac{(l+\frac{3}{2})^2}{4\alpha^2}\Big]^{\frac{1}{2}}}{\frac{l+\frac{3}{2}}{2\alpha}} \\
=& \frac{(1+\frac{3}{2})^{\frac{1}{2}}}{(l+\frac{3}{2}}[l+\frac{5}{2}-l-\frac{3}{2}]^{\frac{1}{2}} \\
=& \frac{1}{(1+\frac{3}{2})^{\frac{1}{2}}}
\end{aligned} \tag{36}
$$

So (3) is verified.

The critical step in getting Wallis' formula is the assertion that:

$$
\lim_{l\to\infty}\frac{\langle H\rangle^l_{\min}}{E_{0,l}} = \lim_{l\to\infty}\frac{(l+1)^2}{(l+\frac{3}{2})}\Big[\frac{\Gamma(l+1)}{\Gamma(l+\frac{3}{2})}\Big]^2 = 1 \tag{37}
$$

This is given without proof and amounts to the assertion that $\frac{\Gamma(l+1)}{\Gamma(l+\frac{3}{2})}$ is of order $\frac{1}{\sqrt{l}}$ when $l$ is large. This is by no means obvious. Clearly since $\frac{(l+1)^2}{(l+\frac{3}{2})}$ is of order $l$ the product in (37) will approach 1 as long as $\frac{\Gamma(l+1)}{\Gamma(l+\frac{3}{2})}$ is of order $\frac{1}{\sqrt{l}}$. Using Mathematica or Matlab you can gain confidence that the limit is 1 but for an analytical proof one needs an asymptotic formula for the ratio of two Gamma functions. Such a formula exists and is due to Tricomi and Erdelyi [6] and it is as follows :

$$
\frac{\Gamma(z+\alpha)}{\Gamma(z+\beta)} = z^{\alpha-\beta}\Big[1+\frac{(\alpha-\beta)(\alpha+\beta-1)}{2z}+\mathcal{O}(|z|^{-2}\Big] \tag{38}
$$

Formula (38) holds for large $z$ and bounded $\alpha, \beta$. Note that in our example $\alpha = 1$ and $\beta = \frac{3}{2}$ hence we get the leading factor in (38) of $\frac{1}{\sqrt{l}}$. Using Stirling's series:

$$
\Gamma(n) \sim e^{-n}n^{n-\frac{1}{2}}\sqrt{2\pi}\Big(1+\frac{1}{12n}+\frac{1}{288n^2}+\dots\Big) \tag{39}
$$

one can also get the critical $\frac{1}{\sqrt{l}}$ factor. If you try to use the basic properties of the Gamma function and the "sandwich" principle it is not possible to get both sides approaching 1, hence a more sophisticated estimate process like (38) is needed.

We are now in the home straight. All we need to do is expand the Gamma functions in (37).

The fundamental relationship is this:

$$
\begin{aligned}
\Gamma(l+\frac{3}{2}) =&(l+\frac{1}{2})\,\Gamma(l+\frac{1}{2})\\
=&(l+\frac{1}{2})(l-\frac{1}{2})\,\Gamma(l-\frac{1}{2})\\
=&(l+\frac{1}{2})(l-\frac{1}{2})(l-\frac{3}{2})\,\Gamma(l-\frac{3}{2})\\
&\dots\\
=&\frac{(2l+1)}{2}\frac{(2l-1)}{2}\frac{(2l-3)}{2}\dots\frac{5}{2}\frac{3}{2}\sqrt{\pi}
\end{aligned}
\tag{40}
$$

Hence (37) becomes:

$$
\lim_{l\to\infty}\frac{(l+1)^2}{(l+\frac{3}{2})}\Big[\frac{\Gamma(l+1)}{\Gamma(l+\frac{3}{2})}\Big]^2 = \lim_{l\to\infty}\frac{1}{(l+\frac{3}{2})}\Big[\frac{(l+1)!}{\frac{(2l+1)}{2}\frac{(2l-1)}{2}\frac{(2l-3)}{2}\dots\frac{5}{2}\frac{3}{2}\sqrt{\pi}}\Big]^2 = 1 \tag{41}
$$

Rewriting (41) we get Wallis' formula:

$$
\frac{\pi}{2} = \lim_{l\to\infty}\Pi_{j=1}^{l+1}\frac{(2j)(2j)}{(2j+1)(2j-1)} \tag{42}
$$

## 3 Observations

Once you appreciate the form of the trial function used in the applying the Hamiltonian it is clear that a Gamma function will arise and that in turn leads to $\pi$. Nevertheless, to get Wallis' formula the limit in (37) is critical and could be said to reflect purely circular orbits. What is rather miraculous is that the critical ratio is of order $\frac{1}{\sqrt{l}}$ because this is what ensures that the limit in (37) is 1 rather than something else and hence ensures that Wallis' formula arises.

## 4 Appendix

Orthonormality of associated Legendre polynomials

We need to prove the following:

$$
\int_{-1}^{1} P_k^m(x)\,P_l^m(x)\,dx = \frac{2(l+m)!}{(2l+1)(l-m)!}\delta_{k,l} \tag{43}
$$

where $\delta_{k,l}$ is the Kronecker delta ie $\delta_{k,l}=1$ if $k=l$ and 0 otherwise.

The associated Lengendre polynomials have the following form (which is a generalisation of Rodrigue's formula):

$$
P_l^m(x) = (1-x^2)^{\frac{m}{2}}\frac{d^mP_l(x)}{dx^m} \tag{44}
$$

fpr $l, m = 0, 1, 2, \ldots$

Rodrigue's formula gives us:

$$P_l(x) = \frac{1}{2^l l!}\frac{d^l}{dx^l}(x^2-1)^l \tag{45}$$

for $l = 0, 1, 2, \ldots$

Thus:

$$P_l^m(x) = \frac{1}{2^l l!}\,(1-x^2)^{\frac{m}{2}}\,\frac{d^{m+l}}{dx^{m+l}}(x^2-1)^l \tag{46}$$

To work out (43) requires multiple integrations by parts. To this end the first iteration is:

$$\begin{aligned}
L_{kl}^m =& \frac{1}{2^{k+l}k!l!}\int_{-1}^{1}\underbrace{(1-x^2)^m\frac{d^{k+m}}{dx^{k+m}}(x^2-1)^k}_{u}\;\underbrace{d\Big(\frac{d^{l+m-1}}{dx^{l+m-1}}(x^2-1)^l\Big)}_{dv}\\
=& \frac{1}{2^{k+l}k!l!}\underbrace{\left[(1-x^2)^m\frac{d^{k+m}}{dx^{k+m}}(x^2-1)^k\,\frac{d^{l+m-1}}{dx^{l+m-1}}(x^2-1)^l\right]_{-1}^{1}}_{=0}\\
-&\frac{1}{2^{k+l}k!l!}\int_{-1}^{1}\frac{d^{l+m-1}}{dx^{l+m-1}}(x^2-1)^l\times\,d\Big((1-x^2)^m\frac{d^{k+m}}{dx^{k+m}}(x^2-1)^k\Big)\\
=& -\frac{1}{2^{k+l}k!l!}\int_{-1}^{1}\frac{d^{l+m-1}}{dx^{l+m-1}}(x^2-1)^l\times\,d\Big((1-x^2)^m\frac{d^{k+m}}{dx^{k+m}}(x^2-1)^k\Big)
\end{aligned} \tag{47}$$

The next iteration is as follows:

$$\begin{aligned}
L_{kl}^m =& \frac{1}{2^{k+l}k!l!}\int_{-1}^{1}\underbrace{d\Big((1-x^2)^m\frac{d^{k+m}}{dx^{k+m}}(x^2-1)^k\Big)}_{u}\;\underbrace{d\Big(\frac{d^{l+m-2}}{dx^{l+m-2}}(x^2-1)^l\Big)}_{dv}\\
=& \frac{1}{2^{k+l}k!l!}\left[\underbrace{d\Big((1-x^2)^m\frac{d^{k+m}}{dx^{k+m}}(x^2-1)^k\Big)}_{A}\times\underbrace{\frac{d^{l+m-2}}{dx^{l+m-2}}(x^2-1)^l}_{B}\right]_{-1}^{1}\\
+&\frac{(-1)^2}{2^{k+l}k!l!}\int_{-1}^{1}d\Big(\frac{d^{l+m-3}}{dx^{l+m-3}}(x^2-1)^l\Big)\times d\bigg(d\Big((1-x^2)^m\frac{d^{k+m}}{dx^{k+m}}(x^2-1)^k\Big)\bigg)
\end{aligned} \tag{48}$$

The term A in (48) is zero when evaluated at $x = \pm 1$ since it just $(1-x^2)^m\frac{d^{k+m+1}}{dx^{k+m+1}}(x^2-1)^k - 2mx(1-x^2)^{m-1}\frac{d^{k+m}}{dx^{k+m}}(x^2-1)^k$. We repeat this process $l+m$ times and the derivatives of the term with $(x^2-1)^l$ decrease to $\frac{d^0}{dx^0}(1-x^2)^l = (1-x^2)^l$ and the derivative of the term containing $(1-x^2)^m$ increases to $\frac{d^{l+m}}{dx^{l+m}}$. The structure of the pattern is:

$$\int_{-1}^{1} \underbrace{d^j\Big((1-x^2)^m d^{k+m}(x^2-1)^k\Big)}_{u} \times \underbrace{d\Big(d^{l+m-j}(x^2-1)^l\Big)}_{dv} \tag{49}$$

At each iteration the $uv$ term is zero when evaluated at $x = \pm 1$ and we finally arrive at:

$$L_{kl}^m = \frac{(-1)^{l+m}}{2^{k+l}k!l!} \int_{-1}^{1} (x^2-1)^l \, \frac{d^{l+m}}{dx^{l+m}} \left[ (1-x^2)^m \frac{d^{k+m}}{dx^{k+m}} (x^2-1)^k \right] dx \tag{50}$$

To simplify (50) we use Leibnitz's rule for the derivative of a product:

$$\frac{d^{l+m}}{dx^{l+m}} \left[ (1-x^2)^m \frac{d^{k+m}}{dx^{k+m}} (x^2-1)^k \right] = \sum_{r=0}^{l+m} \binom{l+m}{r} \frac{d^r}{dx^r} (1-x^2)^m \times \frac{d^{l+2m+k-r}}{dx^{l+2m+k-r}} (x^2-1)^k \tag{51}$$

Note that $m \leq l$ and $\frac{d^r}{dx^r}(1-x^2)^m$ is non-zero only when $r \leq 2m$ ( $r$ runs from 0 to $l+m$). Furthermore, $\frac{d^{l+2m+k-r}}{dx^{l+2m+k-r}}(x^2-1)^k$ is non-zero only when $l+2m+k-r \leq 2k$ ie $r \geq 2m+l-k$. Since $l \geq k$ we have that $r \leq 2m$ and $r \geq 2m+l-k \geq 2m$ from which we conclude that $r = 2m$ and $l = k$. The result is that the only non-zero terms occurs under those conditions. Thus we have:

$$\sum_{r=0}^{l+m} \binom{l+m}{r} \frac{d^r}{dx^r} (1-x^2)^m \times \frac{d^{l+2m+k-r}}{dx^{l+2m+k-r}} (x^2-1)^k = \binom{l+m}{2m} \frac{d^{2m}}{dx^{2m}} (1-x^2)^m \times \frac{d^{2l}}{dx^{2l}} (-1)^l (1-x^2)^l \tag{52}$$

Therefore:

$$\begin{aligned} L_{kl}^m =& \frac{(-1)^l \delta_{k,l} (-1)^{l+m}}{2^{2l}(l!)^2} \binom{l+m}{2m} \int_{-1}^{1} (x^2-1)^l \frac{d^{2m}}{dx^{2m}} (1-x^2)^m \times \frac{d^{2l}}{dx^{2l}} (1-x^2)^l \, dx \\ =& \frac{(-1)^l \delta_{k,l} \, (-1)^{l+m}}{2^{2l}(l!)^2} \binom{l+m}{2m} \int_{-1}^{1} (-1)^l \, (1-x^2)^l \frac{d^{2m}}{dx^{2m}} (1-x^2)^m \times \frac{d^{2l}}{dx^{2l}} (1-x^2)^l \, dx \\ =& \frac{\delta_{k,l} \, (-1)^{l+m}}{2^{2l}(l!)^2} \binom{l+m}{2m} \int_{-1}^{1} (1-x^2)^l \frac{d^{2m}}{dx^{2m}} (1-x^2)^m \times \frac{d^{2l}}{dx^{2l}} (1-x^2)^l \, dx \end{aligned} \tag{53}$$

Note that the $\delta_{k,l}$ factor expresses the fact that in the summation only those terms with $k = l$ are non-zero.

By the Binomial Theorem $(1-x^2)^l = \sum_{j=0}^{l} \binom{l}{j} (-1)^{l-j} x^{2(l-j)}$ hence:

$$\begin{aligned} \frac{d^{2l}}{dx^{2l}} (1-x^2)^l =& \sum_{j=0}^{l} \binom{l}{j} (-1)^{l-j} \frac{d^{2l}}{dx^{2l}} x^{2(l-j)} \\ =& \binom{l}{0} (-1)^l \frac{d^{2l}}{dx^{2l}} x^{2l} \\ =& (-1)^l (2l!) \end{aligned} \tag{54}$$

Therefore:

$$
\begin{aligned}
L_{kl}^{m} =& \frac{\delta_{k,l}\,(-1)^{l+m}}{2^{2l}(l!)^2}\,\frac{(l+m)!}{(l-m)!\,(2m)!}\,(-1)^l(2l!)\,(-1)^m(2m)!\int_{-1}^{1}(-1)^l(1-x^2)^l\,dx \\
=& \frac{\delta_{k,l}}{2^{2l}(l!)^2}\,\frac{(l+m)!\,(2l)!}{(l-m)!}\,\int_{-1}^{1}(1-x^2)^l\,dx
\end{aligned}
\tag{55}
$$

In the integral in (55) we make the substiution $x = \cos\theta$ and we are led to a recurrence relation:

$$
\begin{aligned}
I_{2k+1} =& \int_0^\pi \sin^{2l+1}\theta\,d\theta \\
=& \int_0^\pi \underbrace{\sin^{2l}\theta}_{u}\,\underbrace{\sin\theta\,d\theta}_{dv} \\
=& \underbrace{\Big[-\cos\theta\,\sin^{2l}\theta\Big]_0^\pi}_{0} + \int_0^\pi \cos\theta\,2l\sin^{2l-1}\theta\,\cos\theta\,d\theta \\
=& 2l\int_0^\pi \sin^{2l-1}\theta\,(1-\sin^2\theta)\,d\theta \\
=& 2lI_{2k-1} - 2lI_{2l+1}
\end{aligned}
\tag{56}
$$

Hence we get:

$$
\begin{aligned}
I_{2k+1} =& \frac{2l}{2l+1}I_{2k-1} \\
=& \frac{2l}{2l+1}\,\frac{2l-2}{2l-1}\,I_{2k-3} \\
=& \frac{2l}{2l+1}\,\frac{2l-2}{2l-1}\,\frac{2l-4}{2l-3}I_{2k-5} \\
=& \dots \\
=& \frac{2l}{2l+1}\,\frac{2(l-1)}{2l-1}\,\frac{2(l-2)}{2l-3}\dots\frac{2}{3}I_1 \\
=& \frac{2l}{2l+1}\,\frac{2(l-1)}{2l-1}\,\frac{2(l-2)}{2l-3}\dots\frac{2}{3}\times 2 \\
=& \frac{2^l l!}{(2l+1)(2l-1)(2l-3)\dots 3}\times 2 \\
=& \frac{2l+1l!}{\frac{(2l+1)!}{2^l l!}} \\
=& \frac{2^{2l+1}(l!)^2}{(2l+1)!}
\end{aligned}
\tag{57}
$$

where $I_1 = \int_0^\pi \sin\theta\,d\theta = 2$ was used.

Finally, we have that:

$$
\begin{aligned}
L_{kl}^{m} =& \frac{\delta_{k,l}}{2^{2l}(l!)^2}\frac{(l+m)!\,(2l)!}{(l-m)!}\int_{-1}^{1}(1-x^2)^l\,dx \\
=& \frac{\delta_{k,l}}{2^{2l}(l!)^2}\,\frac{(l+m)!\,(2l)!}{(l-m)!}\,\frac{2^{2l+1}(l!)^2}{(2l+1)!} \\
=& \frac{2\,(l+m)!}{(2l+1)\,(l-m)!}\,\delta_{k,l}
\end{aligned}
\tag{58}
$$

# 5 References


[1] Tamar Friedmann and C R Hagen,"Quantum mechanical derivation of the Wallis formula for Pi", Journal of Mathematical Physics, 56 , 112101 (2015); doi: 10.1063/1.4930800, `https://arxiv.org/abs/1510.07813v2`

[2] Ignacio Cortese and J Antonio Garcia,"Wallis formula from the harmonic oscillator", `https://arxiv.org/abs/1709.01214v1`

[3] Claude Cohen-Tannoudji, Bernard Diu, Franke Laloë, "Quantum Mechanics, Volume 1",Wiley, 1997.

[4] Ruel V Churchill, "Fourier Series and Boundary Value Problems, Second Edition", McGraw Hill, 1963.

[5] Albert Messiah, "Quantum Mechanics - Two Volumes Bound as One", Dover, 1999.

[6] F G Tricomi and A Erdelyi, "The asymptotic expansion of a ratio of Gamma functions",Pacific J. Math. 1 (1951), 133-142, `https://projecteuclid.org/download/pdf_1/euclid.pjm/1102613160`


# 6 History

Created

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