Quantum Mechanical Derivation of the Wallis Formula for π

Tamar Friedmann[1]

Department of Mathematics and Department of Physics and Astronomy
University of Rochester, Rochester, N.Y. 14627

C. R. Hagen[2]

Department of Physics and Astronomy
University of Rochester, Rochester, N.Y. 14627

Abstract

A famous pre-Newtonian formula for π is obtained directly from the variational approach to the spectrum of the hydrogen atom in spaces of arbitrary dimensions greater than one, including the physical three dimensions.

The formula for π as the infinite product

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

was derived by John Wallis in 1655 [1] (see also [2]) by a method of successive interpolations. While several mathematical proofs of this formula have been put forth in the past (many just in the last decade) using probability [3], combinatorics and probability [4], geometric means [5], trigonometry [6, 7], and trigonometric integrals [8], there has not been in the literature a derivation of Eq. (1) that originates in physics, specifically in quantum mechanics.

It is the purpose of this paper to show that this formula can in fact be derived from a variational computation of the spectrum of the hydrogen atom. The existence of such a derivation indicates that there are striking connections between well-established physics and pure mathematics [9] that are remarkably beautiful yet still to be discovered.

The Schrödinger equation for the hydrogen atom is given by

$$H\psi = \left(-\frac{\hbar^2}{2m}\nabla^2 - \frac{e^2}{r} \right)\psi = E\psi,$$

with the corresponding radial equation obtained by separation of variables being

$$H(r)R(r) = \left[-\frac{\hbar^2}{2m}\left(\frac{d^2}{dr^2} + \frac{2}{r}\frac{d}{dr} - \frac{\ell(\ell+1)}{r^2} \right) - \frac{e^2}{r} \right]R(r) = ER(r).$$

Using the trial wave function

$$\psi_{\alpha\ell m} = r^\ell e^{-\alpha r^2} Y_\ell^m(\theta, \phi), \tag{2}$$

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[1]Email address: tfriedma@ur.rochester.edu
[2]Email address: hagen@pas.rochester.edu

where $\alpha > 0$ is a real parameter and the $Y_\ell^m(\theta, \phi)$ are the usual spherical harmonics, the expectation value of the Hamiltonian is found to be given by

$$
\begin{aligned}
\langle H \rangle_{\alpha\ell} &\equiv \frac{\langle \psi_{\alpha\ell m} | H(r) | \psi_{\alpha\ell m} \rangle}{\langle \psi_{\alpha\ell m} | \psi_{\alpha\ell m} \rangle} \\
&= \frac{\hbar^2}{2m} \left(\ell + \frac{3}{2} \right) 2\alpha - e^2 \frac{\Gamma(\ell + 1)}{\Gamma(\ell + \frac{3}{2})} \sqrt{2\alpha} \,.
\end{aligned}
$$

As a consequence of the $Y_\ell^m(\theta, \phi)$ in Eq. (2), the function $\psi_{\alpha\ell m}$ is orthogonal to any energy and angular momentum eigenstate that has a value for angular momentum different from ℓ. Therefore the minimization of $\langle H \rangle_\alpha$ with respect to α, namely

$$
\langle H \rangle_{min}^\ell = -\frac{me^4}{2\hbar^2} \frac{1}{(\ell + \frac{3}{2})} \left[\frac{\Gamma(\ell + 1)}{\Gamma(\ell + \frac{3}{2})} \right]^2 , \tag{3}
$$

gives an upper bound for the lowest energy state with the given value of ℓ.

The well-known exact result for the energy levels of hydrogen is

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

where $n_r = 0, 1, 2, \ldots$, so that the lowest energy eigenstate for a given ℓ is the one with $n_r = 0$, namely

$$
E_{0,\ell} = -\frac{me^4}{2\hbar^2} \frac{1}{(\ell + 1)^2} \,.
$$

The accuracy of approximation (3) is thus displayed in the ratio

$$
\frac{\langle H \rangle_{min}^\ell}{E_{0,\ell}} = \frac{(\ell + 1)^2}{(\ell + \frac{3}{2})} \left[\frac{\Gamma(\ell + 1)}{\Gamma(\ell + \frac{3}{2})} \right]^2 ,
$$

a quantity that approaches unity with increasing ℓ [10]. This follows from the fact that in the large ℓ limit the trial solution and the exact result correspond to strictly circular orbits. 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

$$
\frac{[\langle r^4 \rangle_{\alpha\ell} - (\langle r^2 \rangle_{\alpha\ell})^2]^{\frac{1}{2}}}{\langle r^2 \rangle_{\alpha\ell}} = \left(\ell + \frac{3}{2} \right)^{-\frac{1}{2}} ,
$$

which approaches 0 at large ℓ. Both the trial solution orbits and the exact orbits are then identical to those of the Bohr model in the large ℓ limit, as expected from Bohr's correspondence principle.

Therefore one obtains the limit

$$
\lim_{\ell \to \infty} \frac{\langle H \rangle_{min}^\ell}{E_{0,\ell}} = \lim_{\ell \to \infty} \frac{(\ell + 1)^2}{(\ell + \frac{3}{2})} \left[\frac{\Gamma(\ell + 1)}{\Gamma(\ell + \frac{3}{2})} \right]^2 = 1 \,. \tag{4}
$$

This can be seen to lead to the Wallis formula for π. To this end, one invokes the relations $z\Gamma(z) = \Gamma(z+1)$, $\Gamma(\ell+1) = \ell!$, and $\Gamma(\frac{1}{2}) = \sqrt{\pi}$, which bring Eq. (4) to the form

$$\lim_{\ell\to\infty} \left[\frac{(\ell+1)!}{\sqrt{\pi} \cdot \frac{1}{2}\frac{3}{2}\frac{5}{2} \cdots \frac{2\ell+1}{2}} \right]^2 \frac{1}{\ell + \frac{3}{2}} = 1$$

or alternatively

$$\frac{\pi}{2} = \lim_{\ell\to\infty} \prod_{j=1}^{\ell+1} \frac{(2j)(2j)}{(2j-1)(2j+1)} \, , \tag{5}$$

i.e., the Wallis formula for π, as given by Eq. (1).

The analogous computation in arbitrary dimensions also leads to the same formula, with slightly different forms for even and odd dimensions. The radial equation for the hydrogen atom in N dimensions is [11]

$$H_N R = \left[-\frac{\hbar^2}{2m} \left(\frac{d^2}{dr^2} + \frac{N-1}{r}\frac{d}{dr} - \frac{\ell(\ell+N-2)}{r^2} \right) - \frac{e^2}{r} \right] R(r) = ER(r),$$

where $\hbar^2 \ell(\ell + N - 2)$, $\ell = 0, 1, 2, \ldots$ is the spectrum of the square of the angular momentum operator in N dimensions [12, 13]. The same trial wave function as in three dimensions with the $Y_\ell^m(\theta, \phi)$ of Eq. (2) replaced by its N-dimensional analog [11, 12] gives

$$\langle H \rangle_{min}^{N,\ell} = -\frac{me^4}{2\hbar^2} \frac{1}{(\ell + \frac{N}{2})} \left[\frac{\Gamma(\ell + \frac{N-1}{2})}{\Gamma(\ell + \frac{N}{2})} \right]^2 . \tag{6}$$

The exact result [11]

$$E_{n_r,\ell}^N = -\frac{me^4}{2\hbar^2} \frac{1}{(n_r + \ell + \frac{N-1}{2})^2} \, ,$$

in the limit $\ell \to \infty$ with $n_r = 0$ yields

$$\lim_{\ell\to\infty} \frac{\langle H \rangle_{min}^{N,\ell}}{E_{0,\ell}^N} = \lim_{\ell\to\infty} \frac{(\ell + \frac{N-1}{2})^2}{(\ell + \frac{N}{2})} \left[\frac{\Gamma(\ell + \frac{N-1}{2})}{\Gamma(\ell + \frac{N}{2})} \right]^2 = 1. \tag{7}$$

For $N = 2k + 1$, where k is a positive integer (i.e., the case of odd dimensions), this becomes

$$\lim_{\ell\to\infty} \frac{(\ell + k)^2}{(\ell + k + \frac{1}{2})} \left[\frac{\Gamma(\ell + k)}{\Gamma(\ell + k + \frac{1}{2})} \right]^2 = 1$$

which is identical to Eq. (4) once the substitution $\ell \to \ell + k - 1$ is made there, leading again to the Wallis formula. For $N = 2k$, where k is again a positive integer (i.e., the case of even dimensions), Eq. (7) becomes

$$\lim_{\ell\to\infty} \frac{(\ell + k - \frac{1}{2})^2}{(\ell + k)} \left[\frac{\Gamma(\ell + k - \frac{1}{2})}{\Gamma(\ell + k)} \right]^2 = 1,$$

which is readily brought to the form

$$\frac{2}{\pi} = \lim_{\ell\to\infty} \prod_{j=1}^{\ell+1} \frac{(2j-1)(2j+1)}{(2j)(2j)}, \tag{8}$$

the reciprocal form of the Wallis formula.

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[9] For an example of such a connection, see P. T. Landsberg, "A thermodynamic proof of the inequality between arithmetic and geometric mean," Phys. Lett. A **67**, 1 (1978).

[10] For example, the ratio is .849, .906, .932, .978, .998 for $\ell = 0, 1, 2, 10, 100$.

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