Is π really embedded in Quantum Mechanics?

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January 2017

Abstract. In 2015, a paper by Friedmann and Hagen proposed that the Wallis formula for π has a Quantum Mechanical derivation, and is thus embedded in nature. In this paper we discuss why the result is artificial as well as the mathematical reasons why the Wallis Product appeared for the unique case which the authors had chosen. Furthermore, we show why there is no other possible trial wave function which can produce the Wallis Product or any formula for π using their method. Some possible physical reasons for what is occurring are discussed.

Keywords: Variational Principle, Gaussian, Wallis product, π

1. Introduction

Using the variational principle to compute the ground state energy level of the hydrogen atom with the gaussian trial wave function

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

Friedman and Hagen managed to derive the Wallis Formula for π by comparing their result with the exact energy level [1]. Their analysis and result was the basis of their claim that π is embedded in nature and quantum mechanics. However, their claims are unsubstantiated as their result is completely artificial since they do not use the exact wave function of the hydrogen atom, but a gaussian. In fact if their analysis was followed using the exact wave function of the hydrogen atom

$$\psi = r^l \mathrm{e}^{-\alpha r} Y_l^m(\theta, \phi),$$

the result would be exactly 1, since the variational method produces the exact ground state energy level if the exact wave function is used.
We investigate if any formula for π can be produced by using the variational principle with any other trial wave function. Furthermore, we discuss why their chosen gaussian wave function led to the Wallis Formula.

2. Are there other trial wave functions that give the same result?

In order to gain insight as to whether or not other trial wave functions could produce a formula for π, we followed the procedure outlined in [1] with the general trial wave function

$$\psi_{\alpha lm} = r^l e^{-\alpha r^q} Y_l^m(\theta, \phi). \quad (1)$$

Doing so gave the ratio between the general computed ground state energy level and exact ground state energy level as

$$\frac{4(l+1)^2)\left[\Gamma(\frac{2l+2}{q})\right]^2}{(2l+1)(2l+1+q)\Gamma(\frac{2l+1}{q})\Gamma(\frac{2l+3}{q})}, \quad (2)$$

which approaches 1 in the limit of large l, as shown by figure 1 for integers up to 10.

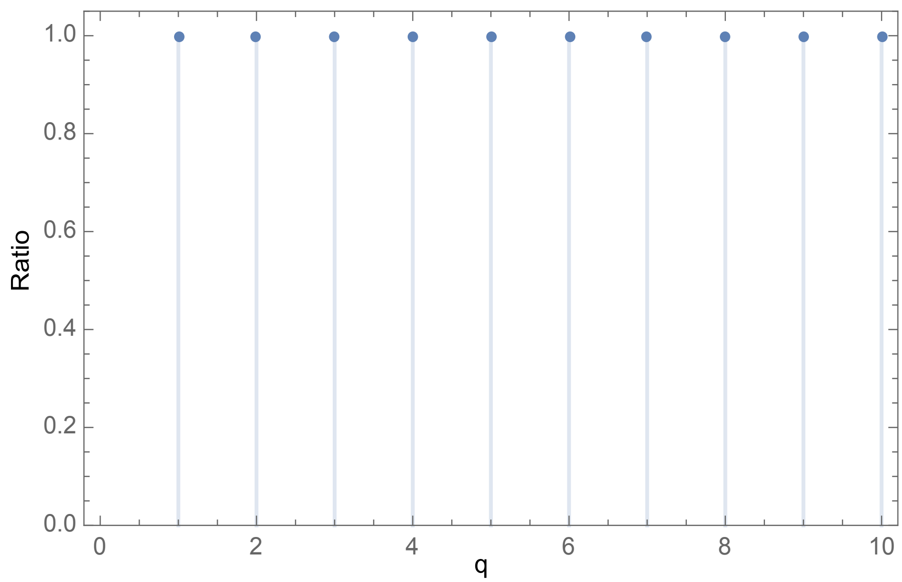

Figure 1. For large values of l, the limiting value of the ratio is always 1 for integer values of q

Now the question is, for what values of q can we get a formula for π by rearranging

$$\lim_{l\to\infty} \frac{4(l+1)^2)\left[\Gamma(\frac{2l+2}{q})\right]^2}{(2l+1)(2l+1+q)\Gamma(\frac{2l+1}{q})\Gamma(\frac{2l+3}{q})} = 1. \quad (3)$$

Since gamma functions are present in 3, the only way to produce π is to have a factor of $\Gamma(l + \frac{1}{2})$ where n is integer [2]. Now on close inspection of 3, this will only ever occur for the case where $q = 2$, the case chosen by the Friedmann and Hagen. We now discuss why this case of the gaussian wave function works mathematically.

3. The Gaussian Wave Function

In Wallis' original proof for the product in 1655, he compared the values of Wallis Integrals,

$$W_n = \int_o^{\frac{\pi}{2}} \sin^n(x)dx, \tag{4}$$

which can be represented using gamma functions depending on the parity of n. So if n is odd, i.e. $n = 2p + 1$, we get

$$W_{2p+1} = \frac{p!\Gamma(\frac{1}{2})}{(2p+1)\Gamma(p+\frac{1}{2})} \tag{5}$$

[2], and if n is even, $n = 2p$, the Wallis integral is

$$W_{2p} = \frac{\Gamma(\frac{1}{2})\Gamma(p+\frac{1}{2})}{2\Gamma(2p+1)} \tag{6}$$

[2].

In his original proof, Wallis expressed the integrals in 5 and 6 as infinite products [3], however we present a revised derivation using the gamma function representations of 6 and 5.

Proof. Firstly, we shall use integration by parts on $W_n = \int_0^{\pi} \sin^n x dx$ as follows:

$$\int_0^{\frac{\pi}{2}} \sin^n x dx = \int_0^{\frac{\pi}{2}} \sin^{n-1} x \sin x dx$$

let $u = \sin^{n-1} x$ and $dv = \sin x dx$ and doing the integration by parts we get:

$$= \Big[-\sin^{n-1}(x)\cos(x) \Big]_0^{\frac{\pi}{2}} + \int_0^{\frac{\pi}{2}} \cos^2(x)(n-1)\sin^{n-2}(x)dx$$

$$= (n-1)\int_0^{\frac{\pi}{2}} \sin^{n-2}(x)\cos^2(x)$$

Since $\cos^2(x) = 1 - \sin^2(x)$,

$$W_n = (n-1)\int_0^{\frac{\pi}{2}} \sin^{n-2}(x)dx - (n-1)\int_0^{\frac{\pi}{2}} \sin^n(x)dx$$

This can be written in the W_n notation as:

$$W_n = (n-1)W_{n-2} - (n-1)W_n$$

$$\therefore \frac{W_n}{W_{n-2}} = \frac{n-1}{n}. \tag{7}$$

Now note that for $x \in [0, \frac{\pi}{2}]$, we have $0 \leq \sin x \leq 1$, which means the following inequalities are true for $x \in [0, \frac{\pi}{2}]$

$$0 \leq \sin^{2n+2} x \leq \sin^{2n+1} x \leq \sin^{2n} x. \tag{8}$$

In terms of W_n notation, the inequalities in equation 8 are:

$$0 \leq W_{2n+2} \leq W_{2n+1} \leq W_2 n. \tag{9}$$

Dividing the inequalities in equation 9 by W_{2n} we get:

$$0 \leq \frac{W_{2n+2}}{W_{2n}} \leq \frac{W_{2n+1}}{W_{2n}} \leq 1. \tag{10}$$

From equation 7, we find that

$$\frac{W_{2n+2}}{W_{2n}} = \frac{2n+1}{2n+2},$$

which means that the inequalities in 10 become

$$0 \leq \frac{2n+1}{2n+2} \leq \frac{W_{2n+1}}{W_{2n}} \leq 1. \tag{11}$$

Now,

$$\lim_{n\to\infty} \frac{2n+1}{2n+2} = 1$$

and

$$\lim_{n\to\infty} 1 = 1,$$

so by the inequality in equation 11 and the squeeze theorem, we get that

$$\lim_{n\to\infty} \frac{W_{2n+1}}{W_{2n}} = 1. \tag{12}$$

Substituting equations 5 and 6 into 12, we get:

$$\begin{aligned} \frac{W_{2n+1}}{W_{2n}} &= \frac{n!\Gamma(\frac{1}{2})}{(2n+1)\Gamma(n+\frac{1}{2})} \times \frac{2\Gamma(2n+1)}{\Gamma(\frac{1}{2})\Gamma(n+\frac{1}{2})} \\ &= \frac{2n!(2n)!}{(2n+1)\left[\Gamma(n+\frac{1}{2})\right]^2} \end{aligned}$$

From 12, it follows that

$$\lim_{n\to\infty} \frac{2n!(2n)!}{(2n+1)\left[\Gamma(n+\frac{1}{2})\right]^2} = 1, \tag{13}$$

and since

$$\Gamma(n+\frac{1}{2}) = \frac{1.3.5...(2n-1)}{2^n}\sqrt{\pi}$$

[2], we can re-write 13 as

$$\lim_{n\to\infty} \frac{2^{n+1} n!(2n)!}{(2n+1)\left[1.3.5...(2n-1)\sqrt{\pi}\right]^2} = 1,$$

which can be re-arranged to give:

$$\prod_{n=1}^{\infty} \frac{(2n)(2n)}{(2n-1)(2n+1)} = \frac{\pi}{2}. \tag{14}$$

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It is evident from the proof above that from a mathematical point of view, the link between the case where $q = 2$ and the Wallis product is that the same gamma function present in the purely mathematical derivation, is also present in the general ratio 2 computed using the variational principle. We are now left to look at whether there is any physical significance to this, or whether the connection is simply purely mathematical.

4. Physical Significance

It is interesting to note that in addition to the many properties of Gaussians, such as that it minimises the uncertainty principle and it is it's own Fourier transform, the Gaussian wave function can produce the Wallis product for π. Although we noted that it is an artificial construct, not actually embedded in nature, it would be of interest to investigate further to see if the Gaussian wave function has any underlying physical reason which lead to this result. Since the formula comes about as taking the limit of large quantum numbers, further investigation could be undertaken looking at coherent states with gaussian wave functions or investigating whether similar results could be found in excited gases or Rydberg atoms.

5. Conclusion

The result published by Friedmann and Hagen was artificially constructed as they used a Gaussian wave function and not the correct wave function for a hydrogen atom. Furthermore, the authors only found a mathematical link between the Gaussian wave function and the Wallis formula, namely that $q = 2$ gives the same gamma function present in the derivation, however no physical reason was found. We suggest further research into the physical significance of this result.

6. References

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[2] Sebah P, Gourdon X. Introduction to the Gamma Function. 2002;.
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