On the quantum mechanical derivation of the Wallis formula for $\pi$

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Abstract

We comment on the Friedmann and Hagen’s quantum mechanical derivation of the Wallis formula for $\pi$. In particular, we demonstrate that not only the Gaussian trial function, used by Friedmann and Hagen, but also the Lorentz trial function can be used to get the Wallis formula. The anatomy of the integrals leading to the appearance of the Wallis ratio is carefully revealed.

Keywords: Variational methods in quantum mechanics, Wallis formula

1. Introduction

Recently Friedmann and Hagen presented an interesting quantum mechanical derivation of the Wallis formula for $\pi$ [1]. Their result follows from comparing the variational principle estimate of the hydrogen atom lowest energy level for a given orbital angular momentum quantum number with the exact quantum mechanical result. The Bohr’s correspondence principle is used to argue that in the limit of large angular momentum quantum numbers the two results should coincide.

Friedmann and Hagen use the Gaussian trial function in their variational calculation. So a question naturally arises whether their recovery of the Wallis formula from these calculations is conditioned by the use of this particular

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form of the trial function. The answer is no because, as we demonstrate below, the Lorentz trial function also enables us to get the Wallis formula for $\pi$ from the variational approach to the spectrum of the hydrogen atom.

The paper is organized as follows. For reader’s convenience, we first reproduce the main steps of the Friedmann and Hagen’s approach. Then we prove an interesting identity for the sum of the corresponding variational energy levels and show how to generalize this identity. The Lorentz trial function is considered in the next section, and we conclude that it also leads to the Wallis formula for $\pi$. Then we try somewhat to demystify the Friedmann and Hagen’s proof of the Wallis formula. Finally, we provide some concluding remarks.

2. Friedmann and Hagen’s approach

The Hamiltonian for the hydrogen atom has the form

$$\hat{H} = -\frac{\hbar^2}{2mr^2} \left[ \frac{\partial}{\partial r} \left( r^2 \frac{\partial}{\partial r} \right) - \hat{l}^2 \right] - \frac{e^2}{r},$$

where

$$\hat{l}^2 = -\frac{1}{\sin^2 \theta} \left[ \sin \theta \frac{\partial}{\partial \theta} \left( \sin \theta \frac{\partial}{\partial \theta} \right) + \frac{\partial^2}{\partial \phi^2} \right]$$

is the square of the angular momentum operator (divided by $\hbar^2$) in spherical coordinates.

For variational estimation of the hydrogen atom energy Friedmann and Hagen use the Gaussian trial function

$$\Psi_{alm} = r^l e^{-\alpha r^2} Y_{lm}(\theta, \phi),$$

where $Y_{lm}(\theta, \phi)$ are the usual spherical harmonics satisfying

$$\hat{l}^2 Y_{lm}(\theta, \phi) = l(l+1) Y_{lm}(\theta, \phi).$$

This trial function has no nodes and thus corresponds to the zero radial quantum number.

Using the orthonormality relation for spherical harmonics and the integral

$$I_m = \int_0^\infty x^m e^{-x^2} = \frac{1}{2} \Gamma \left( \frac{m+1}{2} \right),$$
it is straightforward to get an expectation value of the Hamiltonian \( \hat{H} \) in the quantum state \( |\Psi_{\alpha lm}\rangle \). The result is

\[
< \hat{H} > = \frac{\langle \Psi_{\alpha lm} | \hat{H} | \Psi_{\alpha lm} \rangle}{\langle \Psi_{\alpha lm} | \Psi_{\alpha lm} \rangle} = \frac{\hbar^2 \alpha}{m} \left( l + \frac{3}{2} \right) - e^2 \sqrt{2\alpha} \frac{\Gamma(l+1)}{\Gamma(l+\frac{3}{2})}.
\]

Minimizing this expectation value with respect to \( \alpha \), we get the following variational energy levels of the hydrogen atom:

\[
E_l^{(\alpha)} = -\frac{me^4}{2\hbar^2} \frac{1}{l + \frac{3}{2}} \left[ \frac{\Gamma(l+1)}{\Gamma(l+\frac{3}{2})} \right]^2 = -\frac{me^4}{2\hbar^2} \frac{1}{n + \frac{1}{2}} \left[ \frac{\Gamma(n+1)}{\Gamma(n+\frac{1}{2})} \right]^2,
\]

with \( n = l + 1 \).

It is expected \cite{1} from Bohr’s correspondence principle that for large orbital momentum quantum numbers \( l \) the approximate energy levels (7) should approach the exact quantum mechanical result

\[
E_{0,l} = -\frac{me^4}{2\hbar^2} \frac{1}{(l+1)^2} = -\frac{me^4}{2\hbar^2} \frac{1}{n^2}.
\]

Therefore,

\[
\lim_{n \to \infty} \frac{n^2}{n + \frac{1}{2}} \left[ \frac{\Gamma(n+1)}{\Gamma(n+\frac{1}{2})} \right]^2 = \lim_{n \to \infty} \frac{1}{n + \frac{1}{2}} \left[ \frac{\Gamma(n+1)}{\Gamma(n+\frac{1}{2})} \right]^2 = 1.
\]

Due to the relations \( \Gamma(x+1) = x\Gamma(x) \) and \( \Gamma(1/2) = \sqrt{\pi} \), we have

\[
\frac{1}{n + \frac{1}{2}} \left[ \frac{\Gamma(n+1)}{\Gamma(n+\frac{1}{2})} \right]^2 = \frac{1}{2n+1} \left[ \frac{1 \cdot 2 \cdot 3 \cdots n}{2^{n-1} \cdot \frac{3 \cdot 5 \cdots (2n-1)}{2}} \right]^2 \frac{2}{\pi} = \frac{2 \cdot 2 \cdot 4 \cdot 4 \cdots 2(n-1) \cdot 2(n-1)}{\pi \cdot 1 \cdot 3 \cdot 3 \cdot 5 \cdots (2n-3) \cdot (2n-1) \cdot (2n-1) \cdot 2(n+1)}.
\]

Hence, the limit \cite{9} motivated by the quantum physics of the hydrogen atom implies the Wallis formula for \( \pi \):

\[
\frac{\pi}{2} = \frac{2 \cdot 2 \cdot 4 \cdot 4 \cdot 6 \cdot 6 \cdots}{1 \cdot 3 \cdot 3 \cdot 5 \cdot 5 \cdot 7 \cdots} = \prod_{n=1}^{\infty} \frac{(2n)^2}{(2n-1)(2n+1)}.
\]
3. Some interesting identities

There is still another interesting aspect of the approximate energy levels (7). Having in mind that the exact energy levels (8) resonate with the celebrated Euler result

$$\sum_{n=1}^{\infty} \frac{1}{n^2} = \frac{\pi^2}{6}, \quad (12)$$

one may ask if the analogous simple expression can be obtained for the sum of the series

$$\sum_{n=1}^{\infty} \frac{1}{n + \frac{1}{2}} \left[ \frac{\Gamma(n)}{\Gamma(n + \frac{1}{2})} \right]^2.$$ 

This is really possible! Let us denote

$$a_n = \frac{1}{n + \frac{1}{2}} \left[ \frac{\Gamma(n)}{\Gamma(n + \frac{1}{2})} \right]^2. \quad (13)$$

Then

$$\frac{a_n}{a_{n-1}} = \frac{(n - 1)^2}{n^2 - \frac{1}{4}} = \frac{4(n - 1)^2}{4n^2 - 1}, \quad (14)$$

and

$$4n^2a_n = 4(n - 1)^2a_{n-1} + a_n. \quad (15)$$

Applying this recurrence relation again and again, we get

$$4n^2a_n = 4a_1 + a_2 + a_3 + \ldots + a_n. \quad (16)$$

Therefore,

$$s_n = \sum_{i=1}^{n} a_i = 4n^2a_n - 3a_1. \quad (17)$$

As

$$\lim_{n \to \infty} n^2a_n = \lim_{n \to \infty} \frac{1}{n + \frac{1}{2}} \left[ \frac{\Gamma(n + 1)}{\Gamma(n + \frac{1}{2})} \right]^2 = 1, \quad (18)$$

and \(a_1 = \frac{8}{3\pi}\), we obtain

$$\sum_{n=1}^{\infty} \frac{1}{n + \frac{1}{2}} \left[ \frac{\Gamma(n)}{\Gamma(n + \frac{1}{2})} \right]^2 = \lim_{n \to \infty} s_n = 4 - \frac{8}{\pi}. \quad (19)$$
This result can be generalized even further. Let

\[ b_n = \frac{\Gamma(n + m)\Gamma(n + k)}{\Gamma(n + m + \frac{1}{2})\Gamma(n + k + \frac{3}{2})}. \quad (20) \]

Then

\[ \frac{b_n}{b_{n-1}} = \frac{(n + m - 1)(n + k - 1)}{(n + m)(n + k) + \frac{1}{2}(m - k) - \frac{1}{4}}, \quad (21) \]

and

\[ \frac{4(n + m)(n + k)}{2(k - m) + 1} b_n = \frac{4(n - 1 + m)(n - 1 + k)}{2(k - m) + 1} b_{n-1} + b_n. \quad (22) \]

Similarly to the recurrence relation (15), (22) implies

\[ \sum_{i=1}^{n} b_i = \frac{4(n + m)(n + k)}{2(k - m) + 1} b_n - \left[ \frac{4(m + 1)(k + 1)}{2(k - m) + 1} - 1 \right] b_1. \quad (23) \]

But due to (9)

\[ \lim_{n \to \infty} (n + m)(n + k) b_n = \lim_{n \to \infty} \sqrt{\frac{n + m + \frac{1}{2}}{n + k + \frac{3}{2}}} A(n + m)A(n + k) = 1, \quad (24) \]

where

\[ A(n) = \frac{1}{\sqrt{n + \frac{1}{2}}} \frac{\Gamma(n + 1)}{\Gamma(n + \frac{1}{2})}. \]

Therefore, taking the limit \( n \to \infty \) in (23), we get

\[ \sum_{n=1}^{\infty} \frac{\Gamma(n + m)\Gamma(n + k)}{\Gamma(n + m + \frac{1}{2})\Gamma(n + k + \frac{3}{2})} = \frac{4}{2(k - m) + 1} \left[ 1 - \frac{\Gamma(m + 1)\Gamma(k + 1)}{\Gamma(m + \frac{1}{2})\Gamma(k + \frac{3}{2})} \right], \quad (25) \]

where we have simplified the term containing \( b_1 \) by using \( 4(m + 1)(k + 1) - 2(k - m) - 1 = 4 \left( m + \frac{1}{2} \right) \left( k + \frac{3}{2} \right) \), and the \( \Gamma(x + 1) = x\Gamma(x) \) property of the gamma function. When \( m = k = 0 \), this more general relation is reduced to (19). In fact, (25) is valid for any real \( m \) and \( k \).

As we see, not only the Wallis formula is hidden in the quantum-mechanical hydrogen atom, but also the identity (25) which Euler probably had missed to prove, although the Euler result (12) is not contained in it.
4. Lorentz trial function

A pedagogical usefulness of the Lorentz trial function

\[ \Phi(r) = \frac{1}{a^2 + r^2} \]  

was emphasized in [2]. Let us generalize (26) as follows

\[ \Psi_{alm} = \frac{r^l}{(a^2 + r^2)^{l+1}} Y_l^m(\theta, \phi), \]  

and see what will change in the Friedmann and Hagen’s derivation.

Using the integral

\[ I_{m,n} = \int_0^\infty \frac{x^m}{(1 + x^2)^n} \, dx = \frac{1}{2} \frac{\Gamma(\frac{m+1}{2}) \Gamma(n - \frac{m+1}{2})}{\Gamma(n)}, \]  

which can be obtained from

\[ \int_0^{\pi/2} \sin^{2p-1}(\theta) \cos^{2q-1}(\theta) \, d\theta = \frac{1}{2} \frac{\Gamma(p)\Gamma(q)}{\Gamma(p+q)}, \]  

by substitution \( x = \tan \theta \), we can easily find the expectation value of the Hamiltonian (1) with respect to this new trial function:

\[ \langle \hat{H} \rangle = \frac{\hbar^2}{2m} (l + 1) \left( l + \frac{1}{2} \right) \frac{1}{a^2} - \frac{e^2}{a} \frac{1}{l + \frac{1}{2}} \left[ \frac{\Gamma(l + 1)}{\Gamma(l + \frac{1}{2})} \right]^2. \]  

Minimizing it with respect to \( a \), we get the variational energy levels of the hydrogen atom corresponding to the Lorentz trial function:

\[ E_{l}^{(a)} = -\frac{m e^4}{2 \hbar^2} \frac{1}{(l + 1) \left( l + \frac{1}{2} \right)^3} \left[ \frac{\Gamma(l + 1)}{\Gamma(l + \frac{1}{2})} \right]^4 = -\frac{m e^4}{2 \hbar^2} \frac{n - \frac{1}{2}}{n} \left[ \frac{\Gamma(n)}{\Gamma(n + \frac{1}{2})} \right]^4. \]  

Therefore, we expect

\[ \lim_{l \to \infty} \frac{E_{l}^{(a)}}{E_{0,l}} = \lim_{n \to \infty} \frac{n - \frac{1}{2}}{n^3} \left[ \frac{\Gamma(n + 1)}{\Gamma(n + \frac{1}{2})} \right]^4 = 1. \]  

(32)
But (32) and (9) are equivalent, because

\[
\frac{n - \frac{1}{2}}{n^3} \left[ \frac{\Gamma(n+1)}{\Gamma \left( n + \frac{1}{2} \right)} \right]^4 = \left( \frac{n - \frac{1}{2}}{n + \frac{1}{2}} \right)^2 \left( \frac{n + \frac{1}{2}}{\Gamma(n+1)} \right)^2. 
\]

As we see, the Lorentz trial function also can be used to get a quantum mechanical proof of the Wallis formula. However, unlike (19), it doesn’t seem possible to get a closed form for the sum of approximate energy eigenvalues (31). Just for completeness, let us mention that we can calculate approximately this sum by using the following relation [3]:

\[
\sqrt{\frac{x^2 + \frac{1}{2}x + \frac{1}{8} - \frac{1}{128x}}{1 + \frac{1}{2}x + \frac{1}{8}} < \frac{\Gamma(x + 1)}{\Gamma \left( x + \frac{1}{2} \right)} < \sqrt{\frac{x^2 + \frac{1}{2}x + \frac{1}{8}}{1 + \frac{1}{2}x + \frac{1}{8}}. \quad (33)
\]

If we apply the above described procedures to the isotropic quantum harmonic oscillator with the potential energy \( V(r) = \frac{1}{2}m\omega^2r^2 \), nothing notably happens. The exact energy levels (for zero radial quantum number) \( E_{0,l} = \hbar \omega \left( l + \frac{3}{2} \right) \) are reproduced, if we use the Gaussian trial function. Whereas the Lorentz trial function gives the approximate energy levels

\[
E_l^{(a)} = \hbar \omega \sqrt{\frac{(l + 1) \left( l + \frac{1}{2} \right) \left( l + \frac{3}{2} \right)}{l - \frac{1}{2}}},
\]

and in this case we obtain the valid but uninteresting limit

\[
\lim_{l \to \infty} \frac{(l + 1) \left( l + \frac{1}{2} \right)}{(l + \frac{3}{2}) \left( l - \frac{1}{2} \right)} = 1.
\]

5. Magic demystified

At first sight it may appear magical that a classic formula for \( \pi \) is hidden inside the quantum mechanics of the hydrogen atom. Moreover, two very different trial functions both lead to the very same formula. However, on second thought, it becomes clear that the appearance of the Wallis formula in the variational treatment of the hydrogen atom is related to the presence of the Wallis ratio [4]

\[
W_n = \frac{(2n-1)!!}{(2n)!!} = \frac{1}{\sqrt{\pi}} \frac{\Gamma \left( n + \frac{1}{2} \right)}{\Gamma(n+1)}.
\]

\[\text{7}\]
in the relevant integrals, or in the ratios of the relevant integrals.

In case of the Gaussian trial function, the primary source for the Wallis ratio appearance is the integral (34). In particular, the following ratio of the integrals (35) emerges while calculating the expectation value of the potential energy:

\[
\frac{I_{2l+1}}{I_{2l+2}} = \frac{\Gamma(l+1)}{\Gamma\left(l + \frac{3}{2}\right)} = \frac{\Gamma(n)}{\Gamma\left(n + \frac{1}{2}\right)} = \frac{1}{\sqrt{\pi nW_n}}.
\] (35)

The integral (35) itself can be understood on the base of the recurrence relation

\[
I_m = -\frac{1}{2} \int_0^\infty x^{m-1} e^{-x^2} dx = \frac{1}{2} \int_0^\infty e^{-x^2} dx^{m-1} = \frac{m-1}{2} I_{m-2}.
\] (36)

In case of the Lorentz trial function, we have the following normalization integral:

\[
I_{2l+2,2l+2} = \frac{(-1)^{l+1}}{(l+1)(l+2) \cdots (2l+1)} \left. \frac{\partial^{l+1}}{\partial \alpha^{l+1}} \int_0^\infty \frac{dx}{(1 + \alpha x^2)^{l+1}} \right|_{\alpha=1}
\]

\[
= \frac{(-1)^{l+1} l!}{(2l+1)!} \int_0^\infty \left. \frac{dx}{(1 + x^2)^{l+1}} \frac{\partial^{l+1}}{\partial \alpha^{l+1}} \frac{1}{\sqrt{\alpha}} \right|_{\alpha=1} = \frac{1}{2^{2l+1}} \int_0^\infty \frac{dx}{(1 + x^2)^{l+1}}.
\] (37)

It is well known [5] that the rational integral

\[
G_{l+1} = \int_0^\infty \frac{dx}{(1 + x^2)^{l+1}}
\] (38)

is closely related to the Wallis ratio. Namely, writing

\[
\frac{dx}{(1 + x^2)^{l+1}} = \frac{(1 + x^2 - x^2) dx}{(1 + x^2)^{l+1}} = \frac{dx}{(1 + x^2)^l} + \frac{1}{2l} d\left(\frac{1}{(1 + x^2)^l}\right),
\]

and integrating the second term by parts, we get a recurrence relation

\[
G_{l+1} = \frac{2l-1}{2l} G_l = \frac{1}{2^l} \frac{2l(2l-1)}{l} G_l.
\] (39)

Since \( G_1 = \frac{\pi}{2} \), this recurrence relation implies that [5]

\[
G_{l+1} = \frac{1}{2^{2l}} \frac{(2l)! \pi}{l! l!} = \frac{1}{2^{2l}} \frac{\Gamma(2l+1)}{\Gamma(l+1)\Gamma(l+1)} \frac{\pi}{2} = \frac{\pi}{2} W_l.
\] (40)
where the last step follows from the Legendre’s duplication formula for the gamma function applied to $\Gamma(2l + 1)$:

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

Therefore,

$$I_{2l+2,2l+2} = \frac{\pi}{2^{2l+2}} W_l. \quad (41)$$

On the other hand, integral related to the Coulomb potential has the form

$$I_{2l+1,2l+2} = \left[ \frac{(-1)^l}{(l+2)(l+3) \cdots (2l+1)} \frac{\partial^l}{\partial \alpha^l} \int_0^\infty \frac{dx}{(1+\alpha x^2)^{l+2}} \right]_{\alpha=1}$$

$$= \frac{(-1)^l(l+1)!}{(2l+1)!} \int_0^\infty \frac{x dx}{(1+x^2)^{l+2}} \frac{\partial^l}{\partial \alpha^l} \frac{1}{\alpha} \bigg|_{\alpha=1} = \frac{1}{2} (l!)^2 \frac{(2l+2)!}{(2l+1)!}. \quad (42)$$

Using again the Legendre’s duplication formula applied to $\Gamma(2l + 2)$, we get

$$I_{2l+1,2l+2} = \frac{1}{2^{2l+2}} \sqrt{\pi} \frac{\Gamma(l + 1) \Gamma(l + \frac{3}{2})}{\Gamma(l + \frac{5}{2})} = \frac{1}{2^{2l+2}} \frac{1}{(l+\frac{1}{2})} W_l. \quad (43)$$

Therefore,

$$\frac{I_{2l+1,2l+2}}{I_{2l+2,2l+2}} = \frac{1}{l+\frac{1}{2}} \frac{1}{\pi W_l^2}, \quad (44)$$

which makes clear the origin of the squared Wallis ratio in the expectation value of the Coulomb potential energy.

6. Concluding remarks

It is remarkable and fascinating that a purely quantum mechanical proof of the Wallis formula can be given. However, there is no magic here, only certain easy to understand properties of the integrals involved.

Of course, there is no need in the Bohr’s correspondence principle to prove (9). Indeed, Stirling’s series can be used to get

$$\frac{\Gamma(z + \alpha)}{\Gamma(z + \beta)} \sim z^{\alpha-\beta},$$

9
as \( z \to \infty \) (see, for example, [6]). Then
\[
\lim_{l \to \infty} \frac{(l + 1)^2}{l + \frac{3}{2}} \left[ \frac{\Gamma(l + 1)}{\Gamma\left(l + \frac{3}{2}\right)} \right]^2 = \lim_{l \to \infty} \frac{(l + 1)^2}{\left(l + \frac{3}{2}\right) l} = 1
\]
follows quite simply.

In fact, (9) is a particular case of the more general Wendel’s limit [7]
\[
\lim_{x \to \infty} \frac{\Gamma(x + s)}{x^s \Gamma(x)} = 1
\]
valid for any real \( s \) and \( x \).

An other simple way to prove (9) is provided by Kazarinoff’s double inequality [8]
\[
\sqrt{n + \frac{1}{4}} < \frac{\Gamma(n + 1)}{\Gamma\left(n + \frac{1}{2}\right)} < \sqrt{n + \frac{1}{2}}.
\]
Generalizations of the Wendel’s and Kazarinoff’s results produced a vast mathematical literature on bounds for the ratio of two Gamma functions (see, for example, review papers [9, 10, 11]).

Of course, these comments don’t diminish the charm of Friedmann and Hagen’s derivation. No matter how simple the purely mathematical proof of (9) may seem, no one suspected to find Wallis formula for \( \pi \) in hydrogen atom until Friedmann and Hagen revealed this beautiful connection between \( \pi \) and quantum mechanics.

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