Review: Quantum Mechanical Derivation of Wallis's Formula

Summary The paper [1] uses a variational estimate of the energy spectrum of the Coulomb potential to obtain a formula ("Wallis's formula") for π. The key elements the paper uses in deriving this formula seem to be

(1) The variational method for eigenvalue approximation

(2) A specific choice of a trial wave function, that is $\psi_{\alpha\ell m} \propto r^{\ell} e^{-\alpha r^2} Y_l^m$

(3) Insight to compare the variational estimate of the energy with what we expect from an exact solution.

What is important/interesting?
The seemingly obvious reason why this paper is interesting is that it associates two mathematical formalisms which were originally believed to have no relation to one another. Quantum mechanics, already a somewhat mystifying discipline in the eyes of both the public and scientists, is rendered even more strange in its apparent ability to derive non-intuitive arithmetic identities for a famous mathematical constant.

Personal Comment
But to what extent could we claim that the derivation really connects quantum mechanics to Wallis's formula? I think what we really have is a mathematical formalism which is *typically applied to* problems in quantum mechanics, and arguably would never have existed had those problems also not existed, but is fundamentally independent of the so called true nature of quantum mechanics. No where in the derivation does the measurement problem, the uncertainty principle, or the like make an appearance. Instead one could only make such basic quantum phenomena relevant to the work, by overlaying the derivation with additional ideas.

I think what the authors have really shown is that some eigenvalue problems (again, whose physical relevance is justified only through their relevance to quantum theory problems) and their associated approximation methods could be related to the eigenvalue of a mathematical constant and/or a new derivation of a mathematical identity.

Admittedly though, "A Quantum Mechanical Derivation of Wallis's Formula for π" is a much sexier title than "Relating Eiegenvalue problems to a Mathematical Identity".

1 Paper Notes

Before we work through the main derivation, let's review the variational procedure in QM.

1. Choose a trial wave function ψ_α which depends on a free parameter α
2. Compute expectation value of energy $E(\alpha) = \langle\psi_\alpha|H|\psi_\alpha\rangle/\langle\psi_\alpha|\psi_\alpha\rangle$.
3. Compute α_0 for which $E'(\alpha_0) = 0$ and $E''(\alpha_0) > 0$.
4. Estimate the ceiling of ground state energy according to $E_0 \leq E_\alpha$

In the paper, the trial wave function is

$$\psi^m{}_{\alpha\ell} \propto r^\ell e^{-\alpha r^2} Y_\ell^m(\theta,\phi) = R_{\alpha\ell}\, Y_\ell^m(\theta,\phi) \tag{1}$$

We will compute the normalization factor since we do not need the Hamiltonian to do so. We note that we don't need to consider the normalization in θ, ϕ space because Y_ℓ^m is already normalized in this domain. So focusing on the radial part of the wave functions we find

$$\begin{aligned}
\langle \psi^m{}_{\alpha\ell} | \psi^m{}_{\alpha\ell} \rangle &= \int_0^\infty dr\, r^2 r^{2\ell} e^{-2\alpha r^2} \\
&= \int_0^\infty dr\, r\, r^{2\ell+1} e^{-2\alpha r^2} \\
&= \int_0^\infty du\, \frac{1}{4\alpha} \left(\frac{u}{2\alpha}\right)^{\ell+1/2} e^{-u} \\
&= \frac{1}{2(2\alpha)^{\ell+3/2}} \int_0^\infty du\, u^{\ell+3/2-1}\, e^{-u} \\
&= \frac{\Gamma(\ell+3/2)}{2(2\alpha)^{\ell+3/2}}
\end{aligned} \tag{2}$$

Next we consider how the Hamiltonian operates on our trial wave function. Our Hamiltonian in the position basis is

$$H = -\frac{\hbar^2}{2m}\nabla^2 - \frac{e^2}{r}. \tag{3}$$

We can separate our trial wave function into a radial part and an angular part

$$\psi_{\alpha\ell m} \propto R_{\alpha\ell} Y_\ell^m. \tag{4}$$

The Laplacian acting on this trial wave function then yields

$$\begin{aligned}
\nabla^2 \psi_{\alpha\ell m} &\propto \frac{Y_\ell^m}{r^2}\frac{d}{dr}\left(r^2 \frac{d}{dr} R_{\alpha\ell}\right) + \frac{R_{\alpha\ell}}{r^2}\left[\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta \frac{\partial}{\partial\theta} Y_\ell^m\right) + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2} Y_\ell^m\right] \\
&= \frac{Y_\ell^m}{r^2}\frac{d}{dr}\left(r^2 \frac{d}{dr} R_{\alpha\ell}\right) - \frac{\ell(\ell+1)}{r^2} R_{\alpha\ell} Y_\ell^m,
\end{aligned} \tag{5}$$

where in the second equality we used the eigenvalue equation for the spherical harmonic [2]. In this final equation, the spherical harmonic is not operated on and so we may factor it out of our variational estimate. Thus the Hamiltonian acting on our wave function reduces to

$$H \to -\frac{\hbar^2}{2m}\left[\frac{d^2}{dr^2} + \frac{2}{r}\frac{d}{dr} - \frac{\ell(\ell+1)}{r^2} - \frac{e^2}{r}\right], \tag{6}$$

where the trial wave function is now

$$R_{\alpha\ell} = r^\ell e^{-\alpha r^2}. \tag{7}$$

Acting on this trial wave function with each derivative operator, we obtain

$$\begin{aligned}
\frac{d^2}{dr^2}\left(r^\ell e^{-\alpha r^2}\right) &= \frac{d}{dr}\left[e^{-\alpha r^2}\left(\ell r^{\ell-1} - 2\alpha r^{\ell+1}\right)\right] \\
&= e^{-\alpha r^2}\left(\ell(\ell-1) r^{\ell-2} - 2\alpha(2\ell+1) r^\ell + 4\alpha^2 r^{\ell+2}\right)
\end{aligned} \tag{8}$$

$$\frac{1}{r}\frac{d}{dr}\left(e^{-\alpha r^2}\right) = e^{-\alpha r^2}\left(\ell r^{\ell-2} - 2\alpha r^\ell\right) \tag{9}$$

$$-\frac{\ell(\ell+1)}{r^2}e^{-\alpha r^2}r^\ell = e^{-\alpha r^2}\ell(\ell+1)r^{\ell-2} \tag{10}$$

so that in all we find

$$\begin{aligned}\left[\frac{d^2}{dr^2}+\frac{2}{r}\frac{d}{dr}-\frac{\ell(\ell+1)}{r^2}\right]r^\ell e^{-\alpha r^2} &= e^{-\alpha r^2}\left(\ell(\ell-1)r^{\ell-2}-2\alpha(2\ell+1)r^\ell+4\alpha^2r^{\ell+2}\right.\\ &\qquad\left.+2\ell r^{\ell-2}-4\alpha r^\ell-\ell(\ell+1)r^{\ell-2}\right)\\ &= e^{-\alpha r^2}\left(-2\alpha(2\ell+3)r^\ell+4\alpha^2r^{\ell+2}\right).\end{aligned} \tag{11}$$

The expectation value of the kinetic part of the Hamiltonian operator can thus be written as

$$\begin{aligned}\langle R|H_K|R\rangle &= -\frac{\hbar^2}{2m}\int_0^\infty dr\, r^2\, r^\ell\, e^{-2\alpha r^2}\left(-2\alpha(2\ell+3)r^\ell+4\alpha^2r^{\ell+2}\right)\\ &\equiv -\frac{\hbar^2}{2m}\left[-2\alpha(2\ell+3)\Phi_1+4\alpha^2\Phi_2\right]\end{aligned} \tag{12}$$

where we defined

$$\begin{aligned}\Phi_1 &\equiv \int_0^\infty dr\, r^{2\ell+2}e^{-2\alpha r^2}\\ &= \int_0^\infty du\,\frac{1}{4\alpha}\left(\frac{u}{2\alpha}\right)^{\ell+1/2}e^{-u}\\ &= \frac{\Gamma(\ell+3/2)}{2(2\alpha)^{\ell+3/2}}\end{aligned} \tag{13}$$

$$\begin{aligned}\Phi_2 &\equiv \int_0^\infty dr\, r^{2\ell+4}e^{-2\alpha r^2}\\ &= \int_0^\infty du\,\frac{1}{4\alpha}\left(\frac{u}{2\alpha}\right)^{\ell+3/2}e^{-u}\\ &= \frac{\Gamma(\ell+5/2)}{2(2\alpha)^{\ell+3/2}}.\end{aligned} \tag{14}$$

Our result for the expectation value of the Hamiltonian is then

$$\begin{aligned}\langle R|H_K|R\rangle &= -\frac{\hbar^2}{2m}\left[-2\alpha(2\ell+3)\frac{\Gamma(\ell+3/2)}{2(2\alpha)^{\ell+3/2}}+4\alpha^2\frac{\Gamma(\ell+5/2)}{(2\alpha)(2\alpha)^{\ell+3/2}}\right]\\ &= -\frac{\hbar^2}{2m}\left[-2\alpha(2\ell+3)+2\alpha(\ell+3/2)\right]\frac{\Gamma(\ell+3/2)}{2(2\alpha)^{\ell+3/2}}\\ &= \frac{\hbar^2}{2m}(\ell+3/2)\frac{\Gamma(\ell+3/2)}{(2\alpha)^{\ell+1/2}},\end{aligned} \tag{15}$$

where we note that the last line has a denominator with 2α raised to the power of $\ell+1/2$ (not to the $(\ell+3/2)$).

Now, computing the expectation value of the Coulomb interaction via a similar approach, we find

$$\begin{aligned}\langle R|-e^2/r|\rangle &= -\frac{e^2}{r}\int_0^\infty dr r^2 r^{2\ell}e^{-2\alpha r^2}\\ &= \int_0^\infty du\,\frac{1}{4\alpha}\left(\frac{u}{2\alpha}\right)^\ell e^{-u}\\ &= \frac{\Gamma(\ell+1)}{2(2\alpha)^{\ell+1}},\end{aligned} \tag{16}$$

we finally obtain the full (but non-normalized) expectation value of the Hamiltonian

$$\langle R|H|R\rangle = \frac{\hbar^2}{2m}(\ell + 3/2)\frac{\Gamma(\ell+3/2)}{2(2\alpha)^{\ell+1/2}} - e^2\frac{\Gamma(\ell+1)}{2(2\alpha)^{\ell+1}}. \tag{17}$$

With our result for the normalization of the state (noting that the spherical harmonic normalization is automatically 1),

$$\langle R|R\rangle = \frac{\Gamma(\ell+3/2)}{2(2\alpha)^{\ell+3/2}} \tag{18}$$

the normalized expectation value of the energy is

$$\begin{aligned} E_\alpha &= \frac{\langle R|H|R\rangle}{\langle R|R\rangle} \\ &= \frac{\hbar^2}{2m}\left(\ell+3/2\right)2\alpha - e^2\sqrt{2\alpha}\frac{\Gamma(\ell+1)}{\Gamma(\ell+3/2)}. \end{aligned} \tag{19}$$

Now, we need to find the α which minimizes this energy. First computing the derivative w.r.t. α, we have

$$E'_\alpha = \frac{\hbar^2}{m}(\ell+3/2) - \frac{e^2}{\sqrt{2\alpha}}\frac{\Gamma(\ell+1)}{\Gamma(\ell+3/2)}. \tag{20}$$

So that the critical point is

$$2\alpha_0 = \left(\frac{me^2}{\hbar^2}\right)^2\left[\frac{\Gamma(\ell+1)}{\Gamma(\ell+3/2)}\right]^2\frac{1}{(\ell+3/2)^2}. \tag{21}$$

From Eq.(20), we note that the second derivative of E_α is always positive so this value of α indeed defines a local minimum. Inserting this value into Eq.(19) gives us

$$\begin{aligned} E_{\alpha_0} &= -\frac{1}{2}\frac{me^4}{\hbar^2}\left[\frac{\Gamma(\ell+1)}{\Gamma(\ell+3/2)}\right]^2\frac{1}{(\ell+3/2)} \\ &= -\frac{mc^2\alpha_e^2}{2(\ell+3/2)}\left[\frac{\Gamma(\ell+1)}{\Gamma(\ell+3/2)}\right]^2 \end{aligned} \tag{22}$$

where $\alpha_e \equiv e^2/\hbar c$ is the fine structure constant. By the variational theorem, the equation Eq.(22) is our upper bound on the ground state energy for the hydrogen atom.

Now, the key to obtaining the main result of the paper is to compare this estimate with the exact result for the hydrogen atom. From [2] (I think there should be a better and more relevant reference for this), we know that the exact energy spectrum of the hydrogen atom is

$$E_n^{\text{ex.}} = -\frac{mc^2\alpha^2}{2n^2}, \tag{23}$$

where n is the principal quantum number. Now, the paper, for reasons I cannot currently identify (I think I would need to check Shankar or Weinberg for a better Hydrogen atom reference), states that we can compare the variational estimate and the exact formula by taking $n \equiv \ell + 1$. Doing so and taking the ratio of the two formulas, we have

$$\frac{E_{\alpha_0}}{E_{\ell+1}^{\text{ex.}}} = \frac{(\ell+1)^2}{\ell+3/2}\left[\frac{\Gamma(\ell+1)}{\Gamma(\ell+3/2)}\right]^2. \tag{24}$$

The final insight is to show that this formula asymptotes to 1 as ℓ goes to infinity. We can demonstrate this as follows. First, by the definition of the Gamma function and by Stirling's approximation, we know

$$\Gamma(\ell+1) \simeq \sqrt{2\pi\ell}\left(\frac{\ell}{e}\right)^{\ell} \quad (\text{as } \ell \to \infty) \tag{25}$$

Now, by [3], we have that

$$\Gamma(\ell+3/2) = (\ell+1/2)\Gamma(\ell+1/2) = (\ell+1/2)\frac{(2\ell-1)!!}{2^{\ell}}\sqrt{\pi}, \tag{26}$$

where the double factorial refers to a product of every other integer

$$(2\ell-1)!! = 1 \times 3 \times \cdots (2\ell-3) \times (2\ell-1) = \frac{(2\ell)!}{2^{\ell}\ell!}. \tag{27}$$

Considering $(2\ell-1)!!$ in the limit of large ℓ we find

$$\begin{aligned}
(2\ell-1)!! &= \frac{(2\ell)!}{2^{\ell}\ell!} \\
&\simeq \frac{1}{2^{\ell}}\frac{\sqrt{4\pi\ell}\left(\frac{2\ell}{e}\right)^{2\ell}}{\sqrt{2\pi\ell}\left(\frac{\ell}{e}\right)^{\ell}} \\
&= \sqrt{2}\, 2^{\ell}\left(\frac{\ell}{e}\right)^{\ell},
\end{aligned} \tag{28}$$

so that in the large limit Eq.(26) becomes

$$\Gamma(\ell+3/2) \simeq \ell\sqrt{2\pi}\left(\frac{\ell}{e}\right)^{\ell} \tag{29}$$

We can now have the tools to compute Eq.(24) in the large ℓ limit. We find

$$\begin{aligned}
\lim_{\ell\to\infty}\frac{(\ell+1)^2}{\ell+3/2}\left[\frac{\Gamma(\ell+1)}{\Gamma(\ell+3/2)}\right]^2 &= \lim_{\ell\to\infty}\ell\left[\frac{\sqrt{2\pi\ell}\left(\frac{\ell}{e}\right)^{\ell}}{\sqrt{2\pi}\ell\left(\frac{\ell}{e}\right)^{\ell}}\right]^2 \\
&= 1.
\end{aligned} \tag{30}$$

So the identity is established. Now we need only show how this identity is identical to Wallis's Formula for π. Writing out the identity we have

$$1 = \lim_{\ell\to\infty}\frac{(\ell+1)^2}{\ell+3/2}\left[\frac{\Gamma(\ell+1)}{\Gamma(\ell+3/2)}\right]^2 = \lim_{\ell\to\infty}\frac{\Gamma(\ell+2)^2}{\Gamma(\ell+3/2)\Gamma(\ell+5/2)}. \tag{31}$$

Now, inserting the values of $\Gamma(\ell+5/2)$, $\Gamma(\ell+3/2)$ and $\Gamma(\ell+1)$, namely

$$\Gamma(\ell+1) = (l+1)! = \prod_{j=0}^{\ell+1} j \tag{32}$$

$$\Gamma(\ell+3/2) = \frac{(2\ell+1)!!}{2^{\ell+1}}\sqrt{\pi} = \sqrt{\pi}\prod_{j=0}^{\ell+1}\frac{(2j+1)}{2} \tag{33}$$

$$\Gamma(\ell+5/2) = \frac{(2\ell+3)!!}{2^{\ell+2}}\sqrt{\pi} = \frac{\sqrt{\pi}}{2}\prod_{j=0}^{\ell+1}\frac{(2j+3)}{2}, \tag{34}$$

so that Eq.(31) becomes

$$1 = \frac{2}{\pi}\lim_{\ell\to\infty}\prod_{j=0}^{\ell+1}\frac{2j\cdot 2j}{(2j+1)(2j+3)}, \tag{35}$$

or

$$\prod_{j=0}^{\infty}\frac{2j\cdot 2j}{(2j+1)(2j+3)} = \frac{\pi}{2}. \tag{36}$$

Which is indeed Wallis's formula for π.

Extension Problems

(12/19/2015) QM, Variational Principle, and an Identity
In [1], the authors derive Wallis's formula for π using the spectrum the variational principle in quantum mechanics. What mathematical expressions could we derive, if we applied the same technique to the harmonic oscillator spectrum? Namely, we have the Hamiltonian

$$H = -\frac{\hbar^2}{2m}\vec{\nabla}^2 + \frac{1}{2}m\omega^2 r^2 \tag{37}$$

and our trial wave function will be the same as in the paper:

$$\psi_{\alpha lm}(r,\theta,\phi) \propto r^\ell e^{-\alpha r^2} Y_\ell^m(\theta,\phi). \tag{38}$$

As an additional hint, when we isolate only the radial part of the Hamiltonian, we get the eigenvalue equation

$$H(r)R(r) = \left[-\frac{\hbar^2}{2m}\left(\frac{d^2}{dr^2} + \frac{2}{r}\frac{d}{dr} + \frac{l(l+1)}{r^2}\right) + \frac{1}{2}m\omega^2 r^2\right]R(r) \tag{39}$$

From the Coulomb potential analysis we know that

$$\begin{aligned}\langle\psi_{\alpha\ell m}|\psi_{\alpha\ell m}\rangle &= \frac{\Gamma(\ell+3/2)}{2(2\alpha)^{\ell+3/2}} \\ -\frac{\hbar^2}{2m}\langle\psi_{\alpha\ell m}|\vec{\nabla}^2|\psi_{\alpha\ell m}\rangle &= \frac{\hbar^2}{2m}(\ell+3/2)\frac{\Gamma(\ell+3/2)}{(2\alpha)^{\ell+1/2}}\end{aligned} \tag{40}$$

So we need only compute the potential contribution. Doing so, we have

$$\begin{aligned}\langle\psi_{\alpha\ell m}|\frac{1}{2}m\omega^2 r^2|\psi_{\alpha\ell m}\rangle &= \frac{1}{2}m\omega^2\int_0^\infty dr\, r^2 r^{2\ell} e^{-2\alpha r^2} r^2 \\ &= \frac{1}{2}m\omega^2\int_0^\infty dr\, r\, r^{2\ell+3} r^{2\ell} e^{-2\alpha r^2} \\ &= \frac{1}{2}m\omega^2\int_0^\infty \frac{du}{4\alpha}\left(\frac{u}{2\alpha}\right)^{\ell+3/2} e^{-u} \\ &= \frac{1}{2}m\omega^2\frac{1}{2(2\alpha)^{\ell+5/2}}\int_0^\infty du\, u^{\ell+5/2-1} e^{-u}\end{aligned}$$

$$= \frac{1}{2}m\omega^2 \frac{\Gamma(\ell+5/2)}{2(2\alpha)^{\ell+5/2}}. \tag{41}$$

And the normalized estimate is

$$\begin{aligned}\frac{\langle\psi_{\alpha\ell m}|\frac{1}{2}m\omega^2 r^2|\psi_{\alpha\ell m}\rangle}{\langle\psi_{\alpha\ell m}|\psi_{\alpha\ell m}\rangle} &= \frac{1}{2}m\omega^2 \frac{\Gamma(\ell+5/2)}{2(2\alpha)^{\ell+5/2}} \cdot \frac{2(2\alpha)^{\ell+3/2}}{\Gamma(\ell+3/2)} \\ &= \frac{1}{2}m\omega^2 \frac{\Gamma(\ell+5/2)}{\Gamma(\ell+3/2)} \frac{1}{2\alpha} \\ &= \frac{m\omega^2}{4\alpha}(\ell+3/2). \end{aligned} \tag{42}$$

The normalized estimate for the kinetic energy term is

$$-\frac{\hbar^2}{2m} \frac{\langle\psi_{\alpha\ell m}|\vec{\nabla}^2|\psi_{\alpha\ell m}\rangle}{\langle\psi_{\alpha\ell m}|\psi_{\alpha\ell m}\rangle} = \frac{\hbar^2}{2m}(\ell+3/2)2\alpha. \tag{43}$$

Thus, the total energy estimate as a function of α is

$$E(\alpha) = (\ell+3/2)\left[\frac{\hbar^2}{m}\alpha + \frac{m\omega^2}{4\alpha}\right]. \tag{44}$$

Computing the value of α at which this energy is maximized, we have

$$\begin{aligned} 0 = E'(\alpha_0) &= (\ell+3/2)\left[\frac{\hbar^2}{m} - \frac{m\omega^2}{4\alpha_0^2}\right] \quad \Longrightarrow \quad \alpha_0 = \frac{m\omega}{2\hbar} \\ E''(\alpha_0) &= (\ell+3/2)m\omega^2 \frac{1}{2\alpha_0^3} > 0. \end{aligned} \tag{45}$$

Therefore we find

$$\begin{aligned} E(\alpha_0) &= (\ell+3/2)\left[\frac{\hbar^2}{m\omega}\frac{m\omega}{\hbar} + \frac{m\omega^2}{2}\frac{\hbar}{m\omega}\right] \\ &= \hbar\omega(\ell+3/2). \end{aligned} \tag{46}$$

If we identify ℓ with n we see that this is the exact result for the energy levels of the 3D oscillator. Note, we needn't take any limit to reproduce this exact result.

So we did not reproduce any derivation of a fundamental constant or an identity. It seems that the Wallis formula result is only connected to quantum mechanics problems in inverse distance potentials.

References

[1] T. Friedmann and C. Hagen, "Quantum mechanical derivation of the wallis formula for π," *Journal of Mathematical Physics*, vol. 56, no. 11, p. 112101, 2015.

[2] D. J. Griffiths, *Introduction to quantum mechanics*. Pearson Education India, 2005.

[3] E. W. Weisstein, "Double factorial," 2002.