FRACTIONAL PERTURBATION THEORY

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ABSTRACT. In this paper, we present a hybrid Quantum Mechanical variational/perturbative technique using so-called "Fractional" angular momentum eigenfunctions[2]. A result of using these Fractional Spherical Harmonics is that the angular kinetic energy term, $l(l+1)/2mr^2$, in the Hamiltonian becomes, $l_\alpha(l_\alpha+1)/2mr^2$, where we abbreviate, $l_\alpha \equiv l + \alpha$, and where α is presumed small. This forces an alteration of the zero-order radial eigenfunction, apparently allowing for an interplay of energy between the angular and radial energies. To employ this effect in perturbation theory, we follow the same methods as in the standard theory, but use the above mentioned fractional zero-order functions to calculate the required expectation values. After the fractional energy estimate is calculated, we extremize this energy with respect to α, hoping to obtain a more accurate value than the standard theory.

1. INTRODUCTION

We investigate two systems using a new general variational/perturbative technique, which is based on the fractional angular momentum eigenfunctions introduced in the work[2]. In particular, we apply a modified first- and second-order perturbation theory to a perturbed three-dimensional SHO Hamiltonian, and to the fine structure of the Hydrogen atom. In these systems, the "Fractional" functions possess a parameter, α, which labels the non-integer, or non-half-integer, character of the angular momentum states. By generalizing a system to include fractional angular momentum, this parameter can be optimized to find a more accurate value for the perturbative energy estimate. Both of our systems were chosen to have known, exact solutions, so that a comparison of our new method to the standard method can be made. In both of these systems, we find significant improvement in the accuracy of the first-order fractional perturbation theory over the standard perturbation theory. The price paid is in minimizing the energy to evaluate the variational parameter, α. However, in the second-order calculations, we reuse this parameter, and employ the same zero-order solutions. The result is that the fractional, second-order calculation leads to an improvement in the error over that of the standard second-order method of approximately the same ratio as the first-order improvement. Furthermore, since we do not need to extremize the

total energy again, the fractional second-order calculation is just as quick as the standard one, where $\alpha = 0$.

In short, we develop a new perturbation theory, "Fractional Perturbation Theory", where the main ideas are as follows:

(i) Insert a small parameter, "α", to the radial Schrodinger equation, by adding and subtracting it.

(ii) Use regular perturbation theory to obtain the fractional zero-order solutions.

(iii) Minimize the first-order energy with respect to "α" to find the best value, "α_{best}", which gives a better energy estimate, and determines the optimized zero-order basis.

(iv) Use this basis and α_{best} in higher orders, if better accuracy is required.

The general theory of the Fractional Calculus, upon which our fractional zeroth order functions rest, is given in [8]. Other applications of the Fractional Calculus as applied to Quantum Mechanics are given, for instance, in [3],[1],[7], and [6].

2. Method: Fractional Perturbation Theory

Our fractional perturbation theory applies to those Hamiltonians having an angular momentum term. In three-dimensions, we write a general, perturbed, central force Hamiltonian as,

$$H = H_0 + \Delta H \tag{1}$$

$$= \frac{p_r^2}{2m} + \hbar^2 \frac{l(l+1)}{2mr^2} + V(r) + \Delta H$$

$$= \left[\frac{p_r^2}{2m} + \hbar^2 \frac{l_\alpha(l_\alpha+1)}{2mr^2} + V(r) \right] + \left[\hbar^2 \frac{l(l+1) - l_\alpha(l_\alpha+1)}{2mr^2} + \Delta H \right]$$

$$\equiv H_0^{(\alpha)} + \Delta H^{(\alpha)}$$

where now the unperturbed eigenfunctions are the solutions to the new fractional Hamiltonian, (1st braces), and there is a new term in the perturbation, (2nd braces). Note that we define the shorthand, $l_\alpha \equiv l + \alpha$. We assume a small value of α, so that the first perturbed term can be treated as small.

Upon solving for the eigenfunctions and eigenenergies of the new unperturbed, fractional Hamiltonian as,

$$H_0^{(\alpha)}|\psi_0^{(\alpha)}> = E_0^{(\alpha)}|\psi_0^{(\alpha)}> \tag{2}$$

we use first order perturbation theory to find the correction,

$$\Delta E^{(\alpha)} = <\psi_0^\alpha|\Delta H^{(\alpha)}|\psi_0^{(\alpha)}> \tag{3}$$

We then minimize this new energy with respect to α as,

$$\partial_\alpha \left(E_0^{(\alpha)} + \Delta E^{(\alpha)} \right) = 0 \tag{4}$$

Having found this best value of $\alpha = \alpha_{best}$, we find our presumably improved first order calculation as,

$$E = \left(E_0^{(\alpha_{best})} + \Delta E^{(\alpha_{best})} \right) \tag{5}$$

3. Results

3.1. **Perturbed Three-Dimesional SHO.** To begin a first application of fractional perturbation theory, we write an unperturbed three-dimensional, radial SHO Hamiltonian as,

$$H_0 = \frac{p_r^2}{2m} + \hbar^2 \frac{l\,(l+1)}{2mr^2} + \frac{1}{2}m\omega^2 r^2 \tag{6}$$

We next introduce a perturbation, as in the text of Griffiths[5], where the spring constant is altered slightly to $k \to k\,(1+\epsilon)$, where ϵ is small. Then (6) becomes,

$$H = \frac{p_r^2}{2m} + \hbar^2 \frac{l\,(l+1)}{2mr^2} + \frac{1}{2}m\omega^2\,(1+\epsilon)\,r^2 \tag{7}$$

$$= H_0 + \epsilon\frac{1}{2}m\omega^2 r^2$$

$$\equiv H_0 + \Delta H$$

Now it is well-known that the exact solution to the unperturbed (6) has the eigenenergies,

$$E_0 = \hbar\omega\left(n+l+\frac{3}{2}\right) \tag{8}$$

Thus the perturbed Hamiltonian, (7) also has exact energies,

$$E_\epsilon^{(exact)} = \hbar\omega\,(1+\epsilon)^{\frac{1}{2}}\left(n+l+\frac{3}{2}\right) \tag{9}$$

In this section, we compare our first order fractional perturbation theory to the standard perturbation theory as applied to this Hamiltonian, where we have the exact result (9). As suggested in the Methods, we rewrite (7) as,

$$H = \left[\frac{p_r^2}{2m} + \hbar^2\frac{l_\alpha\,(l_\alpha+1)}{2mr^2} + \frac{1}{2}m\omega^2 r^2\right] + \tag{10}$$

$$+ \left[\hbar^2\frac{l\,(l+1) - l_\alpha\,(l_\alpha+1)}{2mr^2} + \epsilon\frac{1}{2}m\omega^2 r^2\right]$$

$$\equiv H_0^{(\alpha)} + \Delta H^{(\alpha)}$$

To facilitate the comparison between the methods, the standard first order perturbation to the energy is easily calculated as,

$$\Delta E^{(std)} = <\psi_{n,l}^{(0)}|\epsilon\frac{1}{2}m\omega^2 r^2|\psi_{n,l}^{(0)}> \tag{11}$$

$$= \epsilon <\psi_{n,l}^{(0)}|V_{sho}|\psi_{n,l}^{(0)}>$$

$$= \frac{\epsilon}{2} <\psi_{n,l}^{(0)}|H_{sho}|\psi_{n,l}^{(0)}>$$

$$= \frac{\epsilon}{2}\hbar\omega\left(n+l+\frac{3}{2}\right)$$

where I have used the Virial Theorem to evaluate the expectation value of V_{sho}. Thus, from (9), the error in the standard first order energy calculation is given by,

$$\Delta_{\epsilon,1}^{(std)} = E_\epsilon^{(exact)} - \left(E_0 + \Delta E^{(std)}\right) = \tag{12}$$

$$= \hbar\omega\left(n+l+\frac{3}{2}\right)\left((1+\epsilon)^{\frac{1}{2}} - \left(1+\frac{\epsilon}{2}\right)\right)$$

We now apply our variational technique to the rearranged, perturbed Hamiltonian (10).

Now as shown in[2], the fractional Spherical Harmonics, $Y_{l_\alpha}^{m_\alpha}(\theta, \varphi)$, satisfy the angular equation,

$$\mathbf{L}^2|Y_{l_\alpha}^{m_\alpha}> = l_\alpha (l_\alpha + 1)|Y_{l_\alpha}^{m_\alpha}> \tag{13}$$

where

$$Y_{l_\alpha}^{m_\alpha}(\theta, \varphi) = P_{l_\alpha}^{m_\alpha}(\theta) e^{im_\alpha \varphi} \tag{14}$$

and where if $l - m$ is even,

$$P_{l_\alpha}^{m_\alpha}(\theta) = \sin^{m_\alpha}(\theta) \sum_{j=0}^{\frac{l-m}{2}} (-1)^j \frac{(2j + l_\alpha + m_\alpha)!}{\left(\frac{l_\alpha + m_\alpha}{2} + j\right)! \left(\frac{l_\alpha - m_\alpha}{2} - j\right)} \frac{\cos^{2j}(\theta)}{(2j)!} \tag{15}$$

and if $l - m$ is odd,

$$P_{l_\alpha}^{m_\alpha}(\theta) = \sin^{m_\alpha}(\theta) \sum_{j=0}^{\frac{l-m-1}{2}} (-1)^j \frac{(2j + l_\alpha + m_\alpha + 1)!}{\left(\frac{l_\alpha + m_\alpha + 1}{2} + j\right)! \left(\frac{l_\alpha - m_\alpha - 1}{2} - j\right)} \frac{\cos^{2j+1}(\theta)}{(2j + 1)!} \tag{16}$$

By use of the Frobenius trial series solution method, the eigen-solution to the unperturbed fractional SHO Hamiltonian of (10) is given by,

$$H_0^{(\alpha)}|R^{(\alpha)}> = \hbar\omega\left(n + l_\alpha + \frac{3}{2}\right)|R^{(\alpha)}> \tag{17}$$

where

$$|R^{(\alpha)}> = r^{l_\alpha} \exp\left(-\frac{1}{2}\frac{m\omega}{\hbar}r^2\right) H_n^{l_\alpha}(r) \tag{18}$$

and where a fractional Hermite polynomial is given by,

$$H_n^{l_\alpha}(r) \equiv \sum_{j=0}^{\frac{n}{2}} c_{2j} r^{2j} \tag{19}$$

$$c_{2j} = (-1)^j \left(\frac{m\omega}{\hbar}\right)^j \frac{\left(l_\alpha + \frac{1}{2}\right)!}{(j)! \left(j + l_\alpha + \frac{1}{2}\right)!} \frac{\left(\frac{n}{2}\right)!}{\left(\frac{n}{2} - j\right)!} c_0 \tag{20}$$

with n even only.

Then with $|Y_{l_\alpha}^{m_\alpha}(\theta, \varphi)>$ and $|R^{(\alpha)}>$ both orthonormal, the fractional, first-order estimate to the full perturbed Hamiltonian is given by,

$$E_\epsilon^{(\alpha)} = <R^{(\alpha)}|<Y_{l_\alpha}^{m_\alpha}|H|Y_{l_\alpha}^{m_\alpha}>|R^{(\alpha)}> \tag{21}$$

$$= \hbar\omega\left(n + l_\alpha + \frac{3}{2}\right) +$$

$$+ <R^{(\alpha)}|\left(\hbar^2\frac{l(l+1) - l_\alpha(l_\alpha + 1)}{2mr^2} + \epsilon\frac{1}{2}m\omega^2 r^2\right)|R^{(\alpha)}>$$

$$\equiv E_0^{(\alpha)} + \Delta E_1^{(\alpha)}$$

This is now minimized with respect to α, according to (4), as

$$\partial_\alpha E_\epsilon^{(\alpha)} \tag{22}$$

$$= \hbar\omega + \partial_\alpha\left(<R^{(\alpha)}|\left(\hbar^2\frac{l(l+1) - l_\alpha(l_\alpha + 1)}{2mr^2} + \epsilon\frac{1}{2}m\omega^2 r^2\right)|R^{(\alpha)}>\right)$$

$$= 0$$

to give the best value, $\alpha = \alpha_{best}$. This is then inserted into (21) to give our best first-order energy caluclation,

$$E_\epsilon^{(\alpha_{best})} = E_0^{(\alpha_{best})} + \Delta E_1^{(\alpha_{best})} \tag{23}$$

The analog to (12) is thus determined,

$$\Delta_{\epsilon,1}^{(frac)} = E_\epsilon^{(exact)} - E_\epsilon^{(\alpha_{best})} \tag{24}$$

$$= \hbar\omega \left(n + l + \frac{3}{2} \right) (1 + \epsilon)^{\frac{1}{2}} - \left(E_0^{(\alpha_{best})} + \Delta E_1^{(\alpha_{best})} \right)$$

The extremization described in (22) looks formidable, but we can use the Feynmann-Hellmann theorem[4] to simplify the expectation values. This theorem states that if the energy is known, we can find various expectation values by differentiating with respect to a parameter as,

$$\frac{d}{d\lambda} E = < \psi\left(\lambda\right) |\partial_\lambda H| \psi\left(\lambda\right) > \tag{25}$$

In our case, we rewrite the unperturbed radial Hamiltonian as,

$$H_0^{(\alpha)} = \frac{p_r^2}{2m} + \hbar^2 \frac{l_\alpha \left(l_\alpha + 1 \right)}{2mr^2} + \frac{1}{2} m\omega^2 r^2 \tag{26}$$

with corresponding eigenenergy,

$$E_0^{(\alpha)} = \hbar\omega \left(n + l_\alpha + \frac{3}{2} \right) \tag{27}$$

Differentiating (26) with respect to the parameter l_α yields,

$$\partial_{l_\alpha} H_0^{(\alpha)} = \frac{\hbar^2 \left(2l_\alpha + 1 \right)}{2m} \frac{1}{r^2} \tag{28}$$

Then employing the Feynmann-Hellmann theorem given in (25), we have for the expectation value,

$$< R^{(\alpha)} | \frac{1}{r^2} | R^{(\alpha)} > = \frac{2m}{\hbar^2 \left(2l_\alpha + 1 \right)} \partial_{l_\alpha} E_0^{(\alpha)} \tag{29}$$

$$= \frac{2m\omega}{\hbar \left(2l_\alpha + 1 \right)}$$

Similarly, we can differentiate (26) with respect to ω to obtain,

$$\partial_\omega H_0^{(\alpha)} = m\omega r^2 \tag{30}$$

and applying the same theorem yields,

$$< R^{(\alpha)} | r^2 | R^{(\alpha)} > = \frac{1}{m\omega} \partial_\omega E_0^{(\alpha)} \tag{31}$$

$$= \frac{\hbar}{m\omega} \left(n + l_\alpha + \frac{3}{2} \right)$$

Inserting these expectation values into (22) and simplifying gives the following equation,

$$\hbar\omega + \partial_\alpha \{ \frac{\hbar^2 \left[l\left(l + 1 \right) - l_\alpha \left(l_\alpha + 1 \right) \right]}{2m} < R^{(\alpha)} | \frac{1}{r^2} | R^{(\alpha)} > + \tag{32}$$

$$+ \frac{1}{2} \epsilon m\omega^2 < R^{(\alpha)} | r^2 | R^{(\alpha)} > \}$$

$$= \hbar\omega \left(1 + \frac{1}{2}\epsilon\right) + \partial_\alpha \left\{ \hbar\omega \frac{l\,(l+1) - l_\alpha\,(l_\alpha + 1)}{(2l_\alpha + 1)} \right\}$$
$$= 0$$

or, performing the differentiation, dividing by $\hbar\omega$, and simplifying, we have for that α which minimizes $E_\epsilon^{(\alpha)}$,

$$\frac{1}{2}\epsilon + \frac{2\alpha\,(\alpha + 2l + 1)}{(2l_\alpha + 1)^2} = 0 \tag{33}$$

Rearranging gives the quadratic,

$$\alpha^2 + (2l+1)\,\alpha + \frac{\epsilon\,(2l+1)^2}{4\,(1+\epsilon)} = 0 \tag{34}$$

with solution,

$$\alpha = -\frac{2l+1}{2} \left(1 \mp \frac{1}{\sqrt{1+\epsilon}}\right) \tag{35}$$

In order that α goes to zero as the perturbation goes to zero, we choose the '$-$' sign and write finally for our best α,

$$\alpha_{best} = -\frac{2l+1}{2} \left(1 - \frac{1}{\sqrt{1+\epsilon}}\right) \tag{36}$$

We now insert α_{best} back into the energy, (21) ,

$$E_0^{(\alpha_{best})} + \Delta E_1^{(\alpha_{best})} = \hbar\omega \left(n + l_{\alpha_{best}} + \frac{3}{2}\right) + \tag{37}$$

$$+\hbar^2 \frac{l\,(l+1) - l_{\alpha_{best}}\,(l_{\alpha_{best}} + 1)}{2m} < R^{(\alpha_{best})}|\frac{1}{r^2}|R^{(\alpha_{best})} > +\epsilon\frac{1}{2}m\omega^2 < R^{(\alpha_{best})}|r^2|R^{(\alpha_{best})} >$$

$$= \hbar\omega \left(n + l_{\alpha_{best}} + \frac{3}{2}\right) + \hbar\omega \frac{l\,(l+1) - l_{\alpha_{best}}\,(l_{\alpha_{best}} + 1)}{(2l_{\alpha_{best}} + 1)} + \frac{1}{2}\epsilon\hbar\omega \left(n + l_{\alpha_{best}} + \frac{3}{2}\right)$$

or

$$E_0^{(\alpha_{best})} + \Delta E_1^{(\alpha_{best})} \tag{38}$$

$$= \hbar\omega \left(1 + \frac{1}{2}\epsilon\right) \left(n + l_{\alpha_{best}} + \frac{3}{2}\right) + \hbar\omega \frac{l\,(l+1) - l_{\alpha_{best}}\,(l_{\alpha_{best}} + 1)}{(2l_{\alpha_{best}} + 1)}$$

Thus, the error in our fractional first-order calculation is given by,

$$\Delta_{\epsilon,1}^{(frac)} = \hbar\omega \left(n + l + \frac{3}{2}\right) (1 + \epsilon)^{\frac{1}{2}} - \left(E_0^{(\alpha_{best})} + \Delta E_1^{(\alpha_{best})}\right) \tag{39}$$

$$= \hbar\omega \left(n + l + \frac{3}{2}\right) \left[(1+\epsilon)^{\frac{1}{2}} - \left(1 + \frac{1}{2}\epsilon\right)\right] - \hbar\omega \left(1 + \frac{1}{2}\epsilon\right) \alpha_{best} -$$

$$- \hbar\omega \frac{l\,(l+1) - l_{\alpha_{best}}\,(l_{\alpha_{best}} + 1)}{(2l_{\alpha_{best}} + 1)}$$

or,

$$\frac{\Delta_{\epsilon,1}^{(frac)}}{\hbar\omega} = \frac{\Delta_{\epsilon,1}^{(std)}}{\hbar\omega} - \left(1 + \frac{1}{2}\epsilon\right) \alpha_{best} - \frac{l\,(l+1) - l_{\alpha_{best}}\,(l_{\alpha_{best}} + 1)}{(2l_{\alpha_{best}} + 1)} \tag{40}$$

When α_{best}, as given by (36), is inserted, this reduces to the following expression,

$$\Delta_{\epsilon,1}^{(frac)} = \hbar\omega\,(n+1) \left[(1+\epsilon)^{\frac{1}{2}} - \left(1 + \frac{\epsilon}{2}\right)\right] \tag{41}$$

independent of l, which shows the superiority of our energy estimate, for all values of ϵ, n, and l. That is, the ratio of the two errors is given by,

$$\frac{\Delta_{\epsilon,1}^{(frac)}}{\Delta_{\epsilon,1}^{(std)}} = \frac{n+1}{n+l+\frac{3}{2}} \tag{42}$$

which is less than one for all quantum numbers. We tabulate below the values of $\Delta_\epsilon^{(frac)}$ and $\Delta_\epsilon^{(std)}$ vs. ϵ for the specific values of $n=2$ and $l=2$. All energies are in units of $\hbar\omega$.

Table I. First-Order Energies for the Perturbed SHO					
ϵ	α_{best}	$E_\epsilon^{(exact)}$	$\Delta_{\epsilon,1}^{(frac)} \cdot 10^{-4}$	$\Delta_{\epsilon,1}^{(std)} \cdot 10^{-4}$	$\Delta_{\epsilon,1}^{(frac)}/\Delta_{\epsilon,1}^{(std)}$
-0.25	0.387	4.763	-269.2	-493.6	0.54545
-0.15	0.212	5.071	-91.37	-167.5	0.54545
-0.05	0.065	5.361	-9.617	-17.63	0.54545
0.05	-0.060	5.636	-9.148	-16.77	0.54545
0.15	-0.169	5.898	-78.58	144.1	0.54545
0.25	-0.264	6.149	-208.98	-383.1	0.54545

We have thus seen the advantage in using the fractional perturbation perturbation in this simple system.

3.2. **Second Order SHO.** We wish to extend this method to 2nd order perturbation theory. The 2nd order energy for our SHO system given by (10) is,

$$E_{n,l}^{(\alpha)} = E_{0;n,l}^{(\alpha)} + E_{1;n,l}^{(\alpha)} + E_{2;n,l}^{(\alpha)} \tag{43}$$

where

$$E_{0;n,l} = < R_{n,l}^{(\alpha)}|H_0^{(\alpha)}|R_{n,l}^{(\alpha)} >= \tag{44}$$
$$= \hbar\omega\left(n + l_\alpha + \frac{3}{2}\right)$$

and where the first-order correction is,

$$E_{1;n,l}^{(\alpha)} = < R_{n,l}^{(\alpha)}|\Delta H^{(\alpha)}|R_{n,l}^{(\alpha)} > \tag{45}$$

$$= < R_{n,l}^{(\alpha)}|\left(\hbar^2\frac{l(l+1)-l_\alpha(l_\alpha+1)}{2mr^2} + \frac{\epsilon}{2}m\omega^2 r^2\right)|R_{n,l}^{(\alpha)} >$$

and where the second-order correction is given by,

$$E_{2;n,l}^{(\alpha)} = \sum_{n_s,l_s} \frac{|< R_{n_s,l_s}^{(\alpha)}|\left(\hbar^2\frac{l(l+1)-l_\alpha(l_\alpha+1)}{2mr^2} + \frac{\epsilon}{2}m\omega^2 r^2\right)|R_{n,l}^{(\alpha)} >|^2}{E_{0;n,l}^{(\alpha)} - E_{0;n_s,l_s}^{(\alpha)}} \tag{46}$$

$$= \sum_{n_s+l_s \neq n+l} \frac{|< R_{n_s,l_s}^{(\alpha)}|\left(\hbar^2\frac{l(l+1)-l_\alpha(l_\alpha+1)}{2mr^2} + \frac{\epsilon}{2}m\omega^2 r^2\right)|R_{n,l}^{(\alpha)} >|^2}{\hbar\omega\left((n+l) - (n_s+l_s)\right)}$$

In making the calculation given in (43) - (46), we use the same value of α_{best}, and the same zero-order base functions, as calculated above in our first-order calculation. This has the side-benefit of simplifying greatly the second-order calculation, since we do not need to extremize again to find a new α_{best}. We tabulate the data, using this technique, in Table II, for $n = l = 2$. Our second-order results in column 4 show the improvement over the standard calculations, which are listed in column 5. Column 6 shows the ratio of the two errors which are similar to the first-order

ratios above for the same state. The sum involved in the second-order calculation was performed using 100 energy levels.

Table II. Second-Order Energies for the Perturbed SHO

ϵ	α_{best}	$E_\epsilon^{(exact)}$	$\Delta_{\epsilon,2}^{(frac)} \cdot 10^{-4}$	$\Delta_{\epsilon,2}^{(std)} \cdot 10^{-4}$	$\Delta_{\epsilon,2}^{(frac)}/\Delta_{\epsilon,2}^{(std)}$
-0.25	0.387	4.763	-35.03	-63.92	0.5480
-0.15	0.212	5.071	-7.073	-12.82	0.5517
-0.05	0.065	5.361	-0.2521	-0.4436	0.5683
0.05	-0.060	5.636	0.2116	0.4167	0.5078
0.15	-0.169	5.898	5.634	10.62	0.5305
0.25	-0.264	6.149	24.86	46.56	0.5340

3.3. **The fine structure of Hydrogen.** We next apply our fractional perturbation theory to the fine structure of Hydrogen. This involves small changes to the energy due to a first-order special relativistic kinematic correction and a spin-orbit coupling between the magnetic moment of the electron and the electromagnetic field of the proton.

Following Griffiths[5], the non-relativistic Hydrogen Hamiltonian is given by,

$$H_0 = \frac{p^2}{2m} - \frac{e^2}{r} \tag{47}$$

The relativistic correction is found by replacing,

$$\frac{p^2}{2m} \rightarrow \sqrt{p^2c^2 + m^2c^4} - mc^2 \approx \frac{p^2}{2m} - \frac{p^4}{8m^3c^2} \tag{48}$$

The second term is then treated as the perturbation,

$$\Delta H_{rel} = -\frac{p^4}{8m^3c^2} \tag{49}$$

The spin-orbit term derives from the interaction,

$$\Delta H_{s.o.} = -\mu \cdot \mathbf{B} \tag{50}$$

where μ is the magnetic moment of the electron and $\mathbf{B}$ is the effective magnetic field encountered by the electron, as caused by the proton. As shown in, e.g., Griffiths[5], this field is parallel to the electrons angular momentum, and is given by,

$$\mathbf{B} = \frac{e}{mc^2r^3}\mathbf{L} \tag{51}$$

It is well-known that the magnetic moment of the electron is anti-parallel to its spin and is given by,

$$\mu = -\frac{e}{2m}\mathbf{S} \tag{52}$$

with $e \equiv |e|$, the magnitude of the electron's charge. Inserting (51) and (52) into (50) yields the spin-orbit perturbation,

$$\Delta H_{s.o.} = \frac{e^2}{2m^2c^2r^3}\mathbf{L} \cdot \mathbf{S} \tag{53}$$

To simplify this, we write for the total angular momentum of the electron, $\mathbf{J} = \mathbf{L}+\mathbf{S}$, and square, giving,

$$\mathbf{L} \cdot \mathbf{S} = \frac{1}{2}\left(\mathbf{J}^2 - \mathbf{L}^2 - \mathbf{S}^2\right) \tag{54}$$

Using this, (53) becomes,

$$\Delta H_{s.o.} = \frac{e^2}{4m^2c^2r^3} \left(\mathbf{J}^2 - \mathbf{L}^2 - \mathbf{S}^2\right) \tag{55}$$

As shown above, we rewrite our perturbed Hamiltonian as,

$$H = \left(\frac{p_r^2}{2m} + \frac{\hbar^2 l\,(l+1)}{2mr^2} - \frac{e^2}{r}\right) + \Delta H_{rel} + \Delta H_{s.o.} \tag{56}$$

$$= \left(\frac{p_r^2}{2m} + \frac{\hbar^2 l_\alpha\,(l_\alpha+1)}{2mr^2} - \frac{e^2}{r}\right) + \hbar^2 \frac{l\,(l+1) - l_\alpha\,(l_\alpha+1)}{2mr^2} + \Delta H_{rel} + \Delta H_{s.o.}$$

$$\equiv \left(\frac{p_r^2}{2m} + \frac{\hbar^2 l_\alpha\,(l_\alpha+1)}{2mr^2} - \frac{e^2}{r}\right) + \Delta H_l + \Delta H_{rel} + \Delta H_{s.o.}$$

where the term in parentheses is now the unperturbed part of the Hamiltonian, and

$$\Delta H_l \equiv \hbar^2 \frac{l\,(l+1) - l_\alpha\,(l_\alpha+1)}{2mr^2} \tag{57}$$

is treated as a perturbation, where again, we have assumed α to be small. The eigenvalues and eigenfunctions of the unperturbed part are found in[2] with fractional eigenfunctions,

$$|n_\alpha, l_\alpha, m_\alpha> = e^{-\frac{\kappa r}{2}} (\kappa r)^{l_\alpha} L_{p_\alpha}^{\kappa_\alpha}(\kappa r) Y_{l_\alpha}^{m_\alpha}(\theta, \varphi) \tag{58}$$

where the fractional Laguerre polynomial is given as,

$$L_{p_\alpha}^{\kappa_\alpha}(\kappa r) = \sum_{j=0}^{n-l-1} (-1)^j \frac{(n_\alpha + l_\alpha)!}{(n-l-1-j)!\,(2l_\alpha+1+j)!\,(j)!} \left(\kappa r^j\right)$$

and where,

$$\kappa = \frac{2me^2}{\hbar^2 n_\alpha} \tag{59}$$

The resulting energy is given by,

$$E_{n,j}^{(0)} = -\frac{me^4}{2\hbar^2 n_\alpha^2} \tag{60}$$

where $n_\alpha \equiv n + \alpha$. Thus the energy to first order is given by taking the expectation value of (56) in one of these states $|n_\alpha, l_\alpha, m_\alpha>$,

$$<H> = -\frac{me^4}{2\hbar^2 n_\alpha^2} + <n_\alpha, l_\alpha, m_\alpha|\Delta H_l|n_\alpha, l_\alpha, m_\alpha> + \tag{61}$$

$$+ <n_\alpha, l_\alpha, m_\alpha|\Delta H_{rel}|n_\alpha, l_\alpha, m_\alpha> + <n_\alpha, l_\alpha, m_\alpha|\Delta H_{s.o.}|n_\alpha, l_\alpha, m_\alpha>$$

$$= -\frac{me^4}{2\hbar^2 n_\alpha^2} + \hbar^2 \frac{l\,(l+1) - l_\alpha\,(l_\alpha+1)}{2m} <r^{-2}> -$$

$$- \frac{1}{8m^3c^2} <p^4> + \frac{e^2}{4m^2c^2} \left(\mathbf{J}^2 - \mathbf{L}^2 - \mathbf{S}^2\right) <r^{-3}>$$

The following results are found in the appendix, where for convenience we switch to atomic units, $(a.u.)$,

$$<r^{-1}> = \frac{1}{n_\alpha^2} \tag{62}$$

$$<r^{-2}> = \frac{1}{\left(l_\alpha + \frac{1}{2}\right) n_\alpha^3} \tag{63}$$

$$< r^{-3} >= \frac{1}{l_\alpha \left(l_\alpha + \frac{1}{2}\right) (l_\alpha + 1) n_\alpha^3} \tag{64}$$

Then we can evaluate the perturbations,

$$< \Delta H_l >= \frac{l(l+1) - l_\alpha (l_\alpha + 1)}{2 \left(l_\alpha + \frac{1}{2}\right) n_\alpha^3} \, (a.u.) \tag{65}$$

$$< \Delta H_{rel.} >= \frac{1}{2n_\alpha^4} \alpha_{f.s.}^2 \left(\frac{3}{4} - \frac{n_\alpha}{l_\alpha + \frac{1}{2}}\right) (a.u.) \tag{66}$$

and

$$< \Delta H_{s.o.} >= \frac{\alpha_{f.s.}^2}{4n_\alpha^3} \frac{< \mathbf{J}^2 - \mathbf{L}^2 - \mathbf{S}^2 >}{l_\alpha \left(l_\alpha + \frac{1}{2}\right) (l_\alpha + 1)} \, (a.u.) \tag{67}$$

where $\alpha_{f.s.}$ is the fine structure constant, and where $< \Delta H_{rel.} >$ is evaluated in the Appendix. We wish to write (65) - (67) in terms of the total angular momentum, j, where by addition of angular momentum we have,

$$j^\pm = l \pm s \tag{68}$$

and where $s = \frac{1}{2}$. Writing for convenience, $j^+ \to j$, and using (68), the perturbation (65) becomes,

$$< \Delta H_l >= \frac{l(l+1) - l_\alpha (l_\alpha + 1)}{2 \left(l_\alpha + \frac{1}{2}\right) n_\alpha^3} \tag{69}$$

$$= -\frac{\alpha}{n_\alpha^3} \frac{(2(j-s) + 1 + \alpha)}{(2(j-s) + 1 + 2\alpha)}$$

or, setting $s \to \frac{1}{2}$,

$$< \Delta H_l >= -\frac{\alpha}{n_\alpha^3} \frac{\left(j_\alpha - \frac{\alpha}{2}\right)}{j_\alpha} \tag{70}$$

where we have set $j_\alpha \equiv j + \alpha$. The corresponding equation for $j_\alpha^- = l_\alpha - 1/2$ is given by,

$$< \Delta H_l >= -\frac{\alpha}{n_\alpha^3} \frac{\left(j_\alpha^- + 1 - \frac{\alpha}{2}\right)}{\left(j_\alpha^- + 1\right)} \tag{71}$$

Using eqn. (68), our expression (66) for $< H_{rel.} >$ becomes,

$$< \Delta H_{rel.} >= \frac{1}{2n_\alpha^4} \alpha_{f.s.}^2 \left(\frac{3}{4} - \frac{n_\alpha}{j_\alpha}\right) (a.u.) \tag{72}$$

The expectation value of the perturbation (67) is also taken in our fractional states. We note that since in these states we have,

$$\mathbf{L}^2 |n_\alpha, l_\alpha, m_\alpha >= l_\alpha (l_\alpha + 1) |n_\alpha, l_\alpha, m_\alpha >$$

so our expression (68) becomes,

$$j_\alpha = l_\alpha + s \tag{73}$$

and this perturbation becomes,

$$< \Delta H_{s.o.} >= \frac{\alpha_{f.s.}^2}{4n_\alpha^3} \frac{((j_\alpha (j_\alpha + 1)) - l_\alpha (l_\alpha + 1) - s(s+1))}{l_\alpha \left(l_\alpha + \frac{1}{2}\right) (l_\alpha + 1)} \tag{74}$$

Simplifying by inserting $l_\alpha = j_\alpha - \frac{1}{2}$ yields,

$$< \Delta H_{s.o.} >= \frac{\alpha_{f.s.}^2}{4n_\alpha^3} \frac{j_\alpha (j_\alpha + 1) - \left(j_\alpha - \frac{1}{2}\right)\left(j_\alpha + \frac{1}{2}\right) - \frac{1}{2}\left(\frac{1}{2} + 1\right)}{\left(j_\alpha - \frac{1}{2}\right) (j_\alpha) \left(j_\alpha + \frac{1}{2}\right)} \tag{75}$$

or,

$$< \Delta H_{s.o.} >= \frac{\alpha_{f.s.}^2}{4n_\alpha^3} \frac{1}{j_\alpha \left(j_\alpha + \frac{1}{2} \right)} \tag{76}$$

Collecting results, we find that the fractional expectation value of the energy of the Hydrogen atom, up to the fine-structure energy, is given by,

$$E_{n,j,\alpha}^{(frac)} = -\frac{1}{2n_\alpha^2} + < \Delta H_l > + < \Delta H_{rel} > + < \Delta H_{s.o.} > \tag{77}$$

$$= -\frac{1}{2n_\alpha^2} - \frac{\alpha}{n_\alpha^3} \frac{\left(j_\alpha - \frac{\alpha}{2} \right)}{j_\alpha} + \frac{1}{2n_\alpha^4} \alpha_{f.s.}^2 \left(\frac{3}{4} - \frac{n_\alpha}{j_\alpha + \frac{1}{2}} \right)$$

In the corresponding expression for $j^- = l - s$, the expression for $< \Delta H_{rel} > + < \Delta H_{s.o.} >$ is identical to that for j^+. Thus, from (71), the fine-structure energy expressed in terms of j^- is given by,

$$E_{n,j^-,\alpha}^{(frac)} = -\frac{1}{2n_\alpha^2} - \frac{\alpha}{n_\alpha^3} \frac{\left(j_\alpha^- + 1 - \frac{\alpha}{2} \right)}{\left(j_\alpha^- + 1 \right)} + \frac{1}{2n_\alpha^4} \alpha_{f.s.}^2 \left(\frac{3}{4} - \frac{n_\alpha}{j_\alpha^- + \frac{1}{2}} \right) \tag{78}$$

Equation (77) can be compared with the standard fine-structure energy given by[5],

$$E_{n,j}^{(std)} = -\frac{1}{2n^2} + \frac{\alpha_{f.s.}^2}{2n^4} \left(\frac{3}{4} - \frac{n}{j + \frac{1}{2}} \right) \tag{79}$$

The numerical comparison is facilitated by using the exact fine-structure formula for hydrogen found using the Dirac equation[5]

$$E_{n,j}^{(exact)} = \alpha_{f.s.}^{-2} \left\{ \left[1 + \left(\frac{\alpha_{f.s.}}{n - \left(j + \frac{1}{2} \right) + \sqrt{\left(j + \frac{1}{2} \right)^2 - \alpha_{f.s.}^2}} \right)^2 \right]^{-\frac{1}{2}} - 1 \right\} \tag{80}$$

Then, after minimizing $E_{n,j,\alpha}^{(frac)}$ to $\alpha = \alpha_{best}$, we calculate,

$$\Delta_{n,j}^{(std)} = E_{n,j}^{(exact)} - E_{n,j}^{(std)} \tag{81}$$

$$\Delta_{n,j}^{(frac)} = E_{n,j}^{(exact)} - E_{n,j,\alpha_{best}}^{(frac)} \tag{82}$$

We now procede to minimize the fractional fine-structure energy, as given in (77), by setting the derivative of this with respect to α to zero. By plotting these energies, we see that the minimum is found at small values of α. A sample plot of this energy is given in Figure 1 for $n = 2$, $j = 3/2$. To find the value of $\alpha = \alpha_{best}$ that minimizes this function, we take advantage of the smallness of α_{best} to approximate the fractional energy as,

$$E_{n,j}^{(frac)} (\alpha) \approx E_{n,j}^{(frac)} (0) + \alpha \partial_\alpha E_{n,j}^{(frac)} (0) + \frac{1}{2} \alpha^2 \partial_\alpha^2 E_{n,j}^{(frac)} (0) \tag{83}$$

Setting to zero the derivative of this function with respect to α gives an approximate value of α_{best} as,

$$\alpha_{best} = -\frac{\partial_\alpha E_{n,j}^{(frac)} (0)}{\partial_\alpha^2 E_{n,j}^{(frac)} (0)} \tag{84}$$
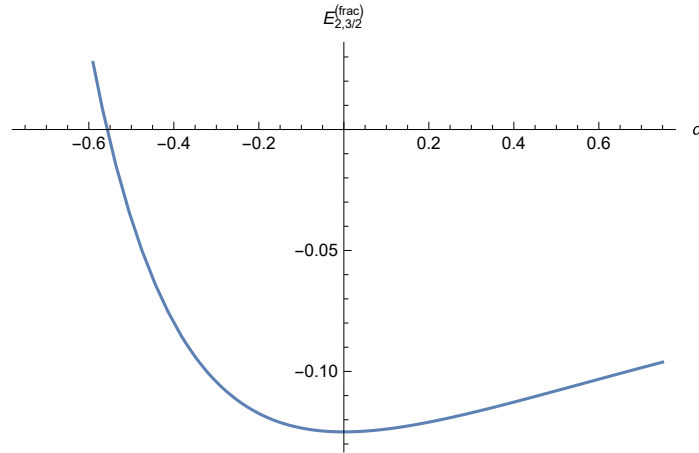
FIGURE 1. $E_{2,3/2}^{(frac)}$ vs. α

In our calculations, we use the following value for the fine structure constant,

$$\alpha_{f.s.} = 7.2973525664 \cdot 10^{-3} \pm \delta\alpha_{f.s.} \qquad (85)$$

where $\delta\alpha_{f.s.} = 1.7 \cdot 10^{-12}$, as obtained from the NIST Reference on Constants, Units, and Uncertainty. The differences in the first-order energies are tabulated below and compared to the exact energies for various values of n and j. The column labeled "δE" represents the approximate uncertainties in the energies due to the uncertainty $\delta\alpha_{f.s.}$. All energies are in atomic units. The last column reveals the degree of advantage in our fractional method. In the interests of space, we have not included all significant figures.

**Table III. Fine Structure Energies**							
n	j	$\alpha_{best}\left(10^{-6}\right)$	$E_{n,j}^{(exact)}$	$\Delta_{n,j}^{(frac)}$	$\Delta_{n,j}^{(std)}$	δE	$\Delta_{n,j}^{(frac)}/\Delta_{n,j}^{(std)}$
1	1/2	-5.32	-0.500006656	$-1.06 \cdot 10^{-10}$	$-1.77 \cdot 10^{-10}$	$3.1 \cdot 10^{-15}$	0.600
2	1/2	-13.3	-0.125002080	$-1.94 \cdot 10^{-11}$	$-5.82 \cdot 10^{-11}$	$9.7 \cdot 10^{-16}$	0.333
2	3/2	-3.07	-0.125000416	$-1.49 \cdot 10^{-12}$	$-2.77 \cdot 10^{-12}$	$1.9 \cdot 10^{-16}$	0.538
3	1/2	-14.8	-0.055556295	$-6.56 \cdot 10^{-12}$	$-1.87 \cdot 10^{-11}$	$3.4 \cdot 10^{-16}$	0.351
3	3/2	-6.66	-0.055555802	$-3.95 \cdot 10^{-13}$	$-1.76 \cdot 10^{-12}$	$1.1 \cdot 10^{-16}$	0.224
3	5/2	-2.11	-0.055555637	$-1.27 \cdot 10^{-13}$	$-2.43 \cdot 10^{-13}$	$3.8 \cdot 10^{-17}$	0.524
4	1/2	-15.1	-0.031250338	$-2.91 \cdot 10^{-12}$	$-7.83 \cdot 10^{-12}$	$1.6 \cdot 10^{-16}$	0.372
4	3/2	-8.22	-0.031250130	$-1.60 \cdot 10^{-13}$	$-9.09 \cdot 10^{-13}$	$6.1 \cdot 10^{-17}$	0.176
4	5/2	-4.02	-0.031250061	$-4.55 \cdot 10^{-14}$	$-1.91 \cdot 10^{-13}$	$2.8 \cdot 10^{-17}$	0.239
4	7/2	-1.61	-0.031250026	$-2.24 \cdot 10^{-14}$	$-4.33 \cdot 10^{-14}$	$1.2 \cdot 10^{-17}$	0.517

All calculations and plots were made using Mathematica[9].

4. DISCUSSION

In the above systems, we find an improvement over the standard perturbative results, at the cost of a new, minimizing calculation. This minimizing involved easy calculations (using Mathematica), with no additional expectation values, e.g., $< r^{-s} >$, required, although we needed to revise these expectation values as computed with fractional functions. However, as derived in the Appendix, the actual

calculation of these generalized expectation values in no way used the actual representation of fractional eigenfunctions.

5. CONCLUSION

The above methods are an application of the the derivation of fractional orbital angular momentum eigenfunctions as constructed in[2]. The manipulations of the Hamiltonian preserve the overall integer character of the angular momentum, since the fractional terms, $\frac{l_\alpha(l_\alpha+1)}{2mr^2}$, are added, but then subtracted from the standard term. In the systems investigated, we saw that the improved accuracy of the fractional first order perturbation results is worth the new required step of minimizing the fractional energy. In both systems, α_{best} was small, thus enabling its easy caluculation. This must be true for applicable systems, since otherwise our new perturbation, $\Delta H \equiv \frac{l(l+1)-l_\alpha(l_\alpha+1)}{2mr^2}$, would in no sense be a small perturbation. Also, in both systems, we saw that the explicit enumeration of the fractional functions is not needed, only that they be assumed square integrable. We hope that the method can be applied to other Hamiltonians possesing orbital angular momentum. Work on extending these methods to systems with spin angular momentum, and also to relativistic perturbation theory, is currently being conducted.

APPENDIX A. VARIOUS EXPECTATION VALUES

We begin by calculation $<\Delta H_{rel}> = -\frac{1}{8m^3c^2}<p^4>$ as was assumed in (66). This term can be put in a more convenient form by noting that, as derived in[2],

$$\left(\frac{\mathbf{p}^2}{2m} - \frac{e^2}{r}\right)|n_\alpha, l_\alpha, m_\alpha> = E_{n_\alpha}|n_\alpha, l_\alpha, m_\alpha> \tag{86}$$

where,

$$E_{n_\alpha} = -\frac{me^4}{2\hbar^2 n_\alpha^2} = -\frac{1}{2n_\alpha^2} \; (a.u.) \tag{87}$$

Then we have,

$$\mathbf{p}^2|n_\alpha, l_\alpha, m_\alpha> = 2m\left(\frac{e^2}{r} + E_{n_\alpha}\right)|n_\alpha, l_\alpha, m_\alpha> \tag{88}$$

and multiplying this by its hermitian conjugate,

$$<n_\alpha, l_\alpha, m_\alpha|\mathbf{p}^4|n_\alpha, l_\alpha, m_\alpha> \tag{89}$$

$$= 4m^2 <n_\alpha, l_\alpha, m_\alpha|\left(\frac{e^2}{r} + E_{n_\alpha}\right)^2|n_\alpha, l_\alpha, m_\alpha>$$

$$= 4m^2\left(E_{n_\alpha}^2 + 2E_{n_\alpha}e^2 <r^{-1}> + e^4 <r^{-2}>\right)$$

where we have abbreviated $<n_\alpha, l_\alpha, m_\alpha|r^s|n_\alpha, l_\alpha, m_\alpha> \equiv <r^s>$. To evaluate the expectation values, we again use the Feynmann-Hellmann relation,

$$\partial_\lambda E_{n_\alpha} = <n_\alpha, l_\alpha, m_\alpha|\partial_\lambda H|n_\alpha, l_\alpha, m_\alpha| > \tag{90}$$

Using

$$H = \frac{p_r^2}{2m} + \hbar^2\frac{l_\alpha(l_\alpha+1)}{2mr^2} - \frac{e^2}{r} \tag{91}$$

and

$$E_{n_\alpha} = -\frac{me^4}{2\hbar^2 n_\alpha^2} = -\frac{1}{2n_\alpha^2} \; (a.u.) \tag{92}$$

we have, setting $\lambda \to e^2$,

$$< \partial_{e^2} H >= - < r^{-1} >, \qquad \partial_{e^2} E_{n_\alpha} = -\frac{me^2}{\hbar^2 n_\alpha^2} \tag{93}$$

or

$$< r^{-1} >= \frac{me^2}{\hbar^2 n_\alpha^2} = \frac{1}{n_\alpha^2} \, (a.u.) \tag{94}$$

To find $< r^{-2} >$, we set $\lambda \to \alpha$, and find,

$$< \partial_\alpha H >= \hbar^2 \frac{2l_\alpha + 1}{2m} < r^{-2} >, \qquad \partial_\alpha E_{n_\alpha} = \frac{me^4}{\hbar^2 n_\alpha^3} \tag{95}$$

or

$$< r^{-2} >= \frac{m^2 e^4}{\hbar^4 \left(l_\alpha + \frac{1}{2}\right) n_\alpha^3} = \frac{1}{\left(l_\alpha + \frac{1}{2}\right) n_\alpha^3} \, (a.u.) \tag{96}$$

Inserting these into (89) yields,

$$< \Delta H_{rel} >= -\frac{1}{8m^3 c^2} < p^4 > \tag{97}$$

$$= -\frac{1}{2mc^2} \left(\left(E_{n_\alpha}^2 + 2 E_{n_\alpha} e^2 < r^{-1} > + e^4 < r^{-2} > \right) \right)$$

$$= -\frac{\alpha_{f.s.}^2}{2} \left(\left(-\frac{1}{2n_\alpha^2}\right)^2 + 2\left(-\frac{1}{2n_\alpha^2}\right)\frac{1}{n_\alpha^2} + \frac{1}{\left(l_\alpha + \frac{1}{2}\right) n_\alpha^3} \right) (a.u.)$$

$$= \frac{\alpha_{f.s.}^2}{2n_\alpha^4} \left(\frac{3}{4} - \frac{n_\alpha}{l_\alpha + \frac{1}{2}} \right) (a.u.)$$

To evaluate $< \Delta H_{s.o} >$, we see from (55) that we need the expectation value $< r^{-3} >$, which cannot be found using the Feynmann-Hellmann relation. However, the following general recursion relation may be derived, in analogy to the standard Kramers relation,

$$\frac{s+1}{n_\alpha^2} < r^s > - (2s+1) < r^{s-1} > + \frac{s}{4} \left[(2l_\alpha + 1)^2 - s^2 \right] < r^{s-2} >= 0 \tag{98}$$

To derive this, start with

$$u''(r) = \left(\frac{l_\alpha (l_\alpha + 1)}{r^2} - \frac{2}{r} + \frac{1}{n_\alpha^2} \right) u(r) \tag{99}$$

and use it to express $\int u r^s u'' dr$ in terms of $< r^s >$, $< r^{s-1} >$, and $< r^{s-2} >$. Then use integration by parts to reduce the second derivative. Thus to find $< r^{-3} >$, we set $s \to -1$ and use (96),

$$< r^{-2} > -\frac{1}{4} \left[(2l_\alpha + 1)^2 - 1 \right] < r^{-3} >= 0 \tag{100}$$

or simplifying,

$$< r^{-3} >= \frac{1}{l_\alpha (l_\alpha + 1)} < r^{-2} >= \frac{1}{l_\alpha \left(l_\alpha + \frac{1}{2}\right)(l+1) n_\alpha^3} \, (a.u) \tag{101}$$

Thus the expectation value of the spin-orbit perturbation is given by,

$$\Delta H_{s.o.} = \frac{\alpha_{f.s.}^2}{4n_\alpha^3} \frac{\left(\mathbf{J}^2 - \mathbf{L}^2 - \mathbf{S}^2\right)}{l_\alpha \left(l_\alpha + \frac{1}{2}\right)(l_\alpha + 1)} \tag{102}$$

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