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New Summation Expressions Involving the Gamma Function

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It is shown how, using standard perturbation theory, one can obtain new summation expressions involving the gamma function.

1. INTRODUCTION

Using standard perturbation theory, if the exact energy of a system is known, one can compare this exact expression and the perturbation expansion for this energy in powers of some small parameter. Equating equal powers of this small parameter sometimes leads, in a conceptually direct way, to new summation expressions.

2. THEORY

In standard perturbation theory [1], it is shown that given the three-dimensional system

$$H = H_0 + h(r) \tag{1}$$

$$H_0 = -\frac{1}{2}\frac{d^2}{dr^2} + \frac{l(l+1)}{2r^2} + V(r) \tag{2}$$

where $V(r)$ is a central potential and $h(r)$ a small central perturbation, then

$$H\Psi_{nl}(r) = E_{nl}\Psi_{nl}(r) \tag{3}$$

$$H_0 R_{nl}(r) = E_{nl}^{(0)} R_{nl}(r) = E_{nl}^{(0)}\big|nl\rangle \tag{4}$$

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and one can write

$$E_{nl} = E_{nl}^{(0)} + \langle nl|h(r)|nl\rangle + \sum_{n'\neq n}^{\infty} \frac{\langle nl|h(r)|n'l\rangle\langle n'l|h(r)|nl\rangle}{E_{nl}^{(0)} - E_{n'l}^{(0)}} + \cdots \tag{5}$$

which is a converging series for appropriate $h(r)$'s. Here $\langle nl|h(r)|n'l\rangle = \int_0^\infty R_{nl}(r)h(r)R_{n'l}(r)r^2\,dr$, etc.

With a little ingenuity, such well-known expressions can be made to yield new mathematical results. A case in point where new infinite sums are obtained is illustrated in what follows.

The simplest new result is

$$\frac{1}{\beta} = \sum_{n'\neq n}^{\infty} \frac{n_>!\Gamma(n_< + \beta + 1)}{n_<!\Gamma(n_> + \beta + 1)} \frac{1}{(n' - n)} \qquad (\beta \neq 0) \tag{6}$$

where $n_>$ ($n_<$) is the bigger (smaller) of n, n'. What makes this an interesting (new) summation rule are the $(n' - n)$ factor, and the fact that it involves *two* parameters (n, β). If β is an integer, Eq. (6) reduces to

$$\frac{1}{\beta} = \sum_{n'\neq n}^{\infty} \frac{n_>!(n_< + \beta)!}{n_<!(n_> + \beta)!} \frac{1}{(n' - n)} \tag{7}$$

If $n = 0$, this reduces to the standard one-parameter expression [2, p. 11]

$$\frac{1}{(n-2)(n-1)!} = \sum_{k=1}^{\infty} \frac{k!}{(n+k-1)!} \tag{8}$$

and in the trivial special case $\beta = 1$, $n = 0$ (where the expression can be easily checked) one obtains

$$1 = \sum_{n'=1}^{\infty} \frac{n'!}{(n'+1)!n'} = \sum_{n'=1}^{\infty} \frac{1}{(n'+1)n'} = \sum_{n'=1}^{\infty} \left(\frac{1}{n'} - \frac{1}{n'+1}\right)$$

3. DERIVATION

Consider the case when, in Eq. (2), $V(r) = \frac{1}{2}r^2$, i.e., one has a three-dimensional harmonic oscillator system. Then [3],

$$R_{nl}(r) = \left\{\frac{2\Gamma(n + l + \frac{3}{2})}{n!}\right\}^{1/2} \frac{r^l e^{-r^2/2}}{\Gamma(l + \frac{3}{2})}\, {}_1F_1\left(-n; l + \frac{3}{2}; r^2\right) \tag{9}$$

Here $n = 0, 1, 2, \ldots$, $l = 0, 1, 2, \ldots$, and the confluent hypergeometric function [2, p. 1045]

$$ {}_1F_1\left(-n;\, l+\frac{3}{2};\, r^2\right) = \sum_{m=0}^{n} \frac{\Gamma(-n+m)\Gamma(l+\frac{3}{2})r^{2m}}{\Gamma(-n)\Gamma(l+\frac{3}{2}+m)m!} \tag{10} $$

is an $n + 1$-term polynomial in r^2.

For this $V(r)$, the unperturbed energy in Eq. (4) is

$$ E_{nl}^{(0)} = 2n + l + \tfrac{3}{2} \tag{11} $$

The bit of ingenuity required here is to use for the central perturbation in Eq. (1)

$$ h(r) = \frac{\alpha}{2r^2} \tag{12} $$

Then

$$ H = -\frac{1}{2}\frac{d^2}{dr^2} + \frac{l(l+1)+\alpha}{2r^2} + \frac{1}{2}r^2 \tag{13} $$

can be written as

$$ H = -\frac{1}{2}\frac{d^2}{dr^2} + \frac{l'(l'+1)}{2r^2} + \frac{1}{2}r^2 \tag{14} $$

where

$$ l' = l + \frac{\alpha}{2l+1} - \frac{\alpha^2}{(2l+1)^3} + \frac{2\alpha^3}{(2l+1)^5} + \cdots \tag{15} $$

Thus, for this $h(r)$, the exact energy in Eqs. (3), (5) is known, namely

$$ E_{nl} = 2n + l' + \tfrac{3}{2} \tag{16} $$

and one has

$$ \begin{aligned} E_{nl} - E_{nl}^{(0)} &= 2n + l' + \frac{3}{2} - \left(2n + l + \frac{3}{2}\right) = l' - l \\ &= \frac{\alpha}{2l+1} - \frac{\alpha^2}{(2l+1)^3} + \frac{2\alpha^3}{(2l+1)^5} + \cdots \\ &= \alpha\langle nl|\frac{1}{2r^2}|nl\rangle + \alpha^2 \sum_{n'\neq n}^{\infty} \frac{\langle nl|\frac{1}{2r^2}|n'l\rangle\langle n'l|\frac{1}{2r^2}|nl\rangle}{2(n-n')} + \cdots \end{aligned} \tag{17} $$

One can then equate equal powers of α to obtain

$$\frac{1}{2l+1} = \langle nl\Big| \frac{1}{2r^2} \Big|nl\rangle \tag{18}$$

$$\frac{1}{(2l+1)^3} = \sum_{n'\neq n}^{\infty} \frac{\langle nl\Big| \frac{1}{2r^2} \Big|n'l\rangle\langle n'l\Big| \frac{1}{2r^2} \Big|nl\rangle}{2(n'-n)} \tag{19}$$

$$\cdots = \cdots$$

To evaluate Eqs. (18), (19) one can use the general expression [4]

$$\begin{aligned} I_{nn'l}(\lambda) &= \langle nl|r^{\lambda}|n'l\rangle \\ &= \left[\frac{\Gamma(n+l+\frac{3}{2})}{n!n'!\Gamma(n'+l+\frac{3}{2})}\right]^{1/2} \frac{\Gamma(\frac{\lambda}{2}+l+\frac{3}{2})\Gamma(n'-\frac{\lambda}{2})}{\Gamma(l+\frac{3}{2})\Gamma(-\frac{\lambda}{2})} \\ &\quad \times {}_3F_2\left(-n, \frac{\lambda}{2}+l+\frac{3}{2}, \frac{\lambda}{2}+1; l+\frac{3}{2}, -n'+\frac{\lambda}{2}+1; 1\right) \qquad (n' \geq n) \end{aligned} \tag{20}$$

where the generalized hypergeometric function ${}_3F_2$ is an $(n+1)$-term polynomial [2, p. 1045] namely

$$\begin{aligned} &= \sum_{p=0}^{n} \frac{\Gamma(-n+p)\Gamma(\frac{\lambda}{2}+l+\frac{3}{2}+p)\Gamma(\frac{\lambda}{2}+1+p)}{\Gamma(-n)\Gamma(\frac{\lambda}{2}+l+\frac{3}{2})\Gamma(\frac{\lambda}{2}+1)} \\ &\quad \times \frac{\Gamma(\frac{l}{2}+\frac{3}{2})\Gamma(-n'+\frac{\lambda}{2}+1)}{\Gamma(\frac{l}{2}+\frac{3}{2}+p)\Gamma(-n'+\frac{\lambda}{2}+1+p)p!} \end{aligned} \tag{21}$$

One notes that if any of the terms $-n$, $\lambda/2 + l + 3/2$, $\lambda/2 + 1$ is zero, the ${}_3F_2$ in Eq. (20) is equal to 1.

The integral expression (20) (with $n = n'$, $\lambda = -2$) confirms the validity of Eq. (18) since

$$\begin{aligned} \langle nl\Big| \frac{1}{2r^2} \Big|nl\rangle &= \frac{1}{2}\frac{1}{n!}\frac{\Gamma(l+\frac{1}{2})\Gamma(n+1)}{\Gamma(l+\frac{3}{2})\Gamma(1)}\, {}_3F_2\left(-n, l+\frac{1}{2}, 0; l+\frac{3}{2}, -n; 1\right) \\ &= \frac{1}{2}\frac{1}{(l+\frac{1}{2})} \end{aligned}$$

where one has used $\Gamma(\beta+1) = \beta\Gamma(\beta)$, and $\Gamma(m+1) = m!$ if m is an integer. This result was recently discussed in an interesting paper [5], where it is obtained using the Hellman–Feynman theorem. Here this result is shown to also follow from Eq. (18) (i.e. equating the linear powers of α) or from Eq. (20) (with $n = n'$, and $\lambda = -2$).

Equation (19) gives the simplest new summation expression. Using Eq. (20) again (this time for $n \neq n'$), one obtains

$$\langle nl| \frac{1}{2r^2} |n'l\rangle = \frac{1}{2}\left[\frac{\Gamma(n+l+\frac{3}{2})}{n!n'!\Gamma(n'+l+\frac{3}{2})}\right]^{1/2} \frac{\Gamma(l+\frac{1}{2})\Gamma(n'+1)}{\Gamma(l+\frac{3}{2})\Gamma(1)} \times {}_3F_2\left(-n, l+\frac{1}{2}, 0; l+\frac{3}{2}, -n'; 1\right)$$

$$= \frac{1}{2}\left(\frac{n'!\Gamma(n+l+\frac{3}{2})}{n!\Gamma(n'+l+\frac{3}{2})}\right)^{1/2} \frac{1}{(l+\frac{1}{2})} \qquad (n' > n) \tag{22}$$

Hence

$$\frac{1}{(2l+1)^3} = \frac{1}{8}\sum_{n'\neq n} \frac{n_>!\Gamma(n_< + l + \frac{3}{2})}{n_<!\Gamma(n_> + l + \frac{3}{2})} \frac{1}{(l+\frac{1}{2})^2(n'-n)} \tag{23}$$

where $n_>$ ($n_<$) is the bigger (smaller) of n, n'. This is just the result of Eq. (6) if we substitute $\beta = l + \frac{1}{2}$.

By comparing the next power of alpha (α^3) in Eq. (17) one obtains a more complicated new double sum expression. For the special case $n = 0$ this reduces to

$$\sum_{k=0}^{\infty} \frac{k!}{\Gamma(k+\beta+2)}\left(\sum_{m=1}^{k}\frac{1}{m}\right) = \frac{1}{\beta^2}\frac{1}{\Gamma(\beta+1)} \qquad (\beta \neq 0) \tag{24}$$

This new result can be added to the known series of the form [6]

$$\sum a_k\left(\sum^{N(k)} b_m\right)$$

If β is an integer, Eq. (24) reduces to

$$\sum_{k=0}^{\infty} \frac{k!}{(k+\beta+1)!}\left(\sum_{m=1}^{k}\frac{1}{m}\right) = \frac{1}{\beta^2}\frac{1}{\beta!} \tag{25}$$

4. CONCLUSIONS

We have used a pedagogically instructive, term-by-term, comparison between the exact expressions for the energy of a particular system and the perturbation expansion for this energy in powers of a parameter, to obtain new summation expressions involving the gamma function. These results reduce to standard expressions in the appropriate limits.

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