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Some New Mathematical Results Obtained Using Closure

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Abstract

Several new mathematical sum rules are derived using closure. Their convergence and other properties are then discussed.

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1. Introduction

The closure formula in one dimension is [1]:

$$\sum_q \phi_q^*(x')\phi_q(x) + \int dE\ \phi_E^*(x')\phi_E(x) = \delta(x-x'), \tag{1}$$

where the sum is over all bound states, and the integral involves the continuum states of any complete set $(\phi_q,\ \phi_E)$. This formula is an indispensable tool in numerous quantum-mechanical manipulations. In this paper we consider a complete, elementary, and extensively-studied, one-dimensional set, that involves only discrete states, namely the eigenfunctions of the infinite square well.

For the case

$$\begin{aligned} V(x) &= 0 \qquad \left(|x| \le \frac{\pi}{2}\right), \\ &= \infty \qquad \left(|x| > \frac{\pi}{2}\right), \end{aligned}$$

the complete set is,

$$\phi_n(x) = \sqrt{\frac{2}{\pi}}\cos nx \qquad (n = 1,\ 3,\ 5...), \tag{2}$$

$$\phi_m(x) = \sqrt{\frac{2}{\pi}}\sin mx \qquad (m = 2,\ 4,\ 6...), \tag{3}$$

the cosines being functions of even parity, and the sines, functions of odd parity.

Equation (1) is illustrated in the Figure as a function of x for this complete set for the case $x' = 0.5$, using the Mathematica software [2], including in the sum the first 14 even parity states (i.e. $n = 1,\ 3,\ 5, \ldots,\ 27$), and the first 14 odd parity states (i.e. $m = 2,\ 4,\ 6, \ldots,\ 28$). This figure illustrates a symmetric, normalized delta function behavior (about $x' = 0.5$ in this instance) and a decaying sinusoidal behavior for $x \neq x'$, that becomes negligible as the number of states included is increased. This complete set involves real, discrete functions, hence, for this case, one may drop the stars and integral over continuum states in eq. (1).

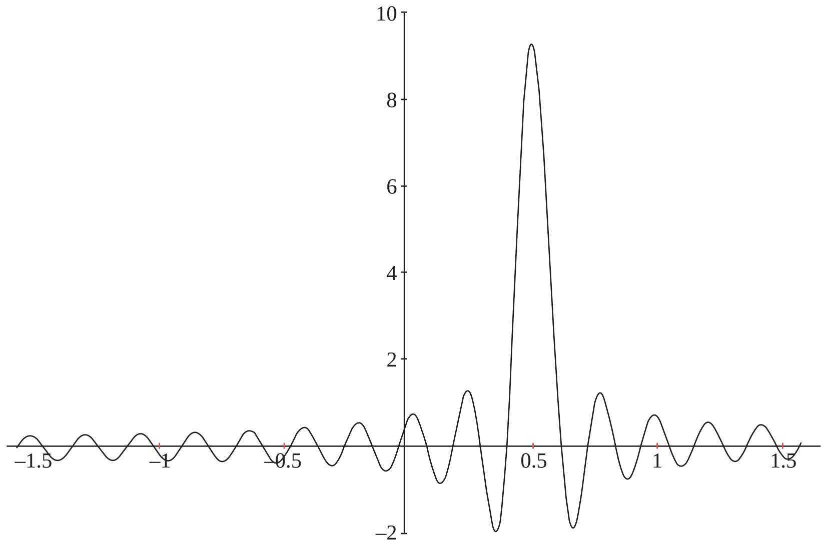

Figure. Plot of eq. (1) for the complete set given by eqs (2), (3), including the complete set given by eqs (2), (3), including the first 14 even and the first 14 odd states, as a function of x for $x' = 0.5$.

Consider two arbitrary operators $\hat{A}, \hat{B}$, and the above basis. Using eq. (1), we have

$$
\begin{aligned}
\int_{-\pi/2}^{\pi/2} \phi_p(x)\hat{A}(x)\hat{B}(x)\phi_p(x)dx &= \int_{-\pi/2}^{\pi/2}\int_{-\pi/2}^{\pi/2} \phi_p(x)\hat{A}(x)\delta(x-x')\hat{B}(x')\phi_p(x')dxdx', \\
= \quad \int_{-\pi/2}^{\pi/2}\int_{-\pi/2}^{\pi/2} \phi_p(x)\hat{A}(x)\sum_q \phi_q(x)\phi_q(x')\hat{B}(x')\phi_p(x')dxdx' \\
= \sum_q \left[\int_{-\pi/2}^{\pi/2} \phi_p(x)\hat{A}(x)\phi_q(x)dx\right]\left[\int_{-\pi/2}^{\pi/2} \phi_q(x')\hat{B}(x')\phi_p(x')dx'\right].
\end{aligned}
\tag{4}
$$

I. Case $\hat{A},\ \hat{B} = x^2$.

If $\hat{A},\ \hat{B} = x^2$, the resulting integrals in the above expression do not mix basis states of different parities:

$$
\begin{aligned}
\int_{-\pi/2}^{\pi/2} \phi_p(x)x^4\phi_p(x)dx &= \sum_q \left[\int_{-\pi/2}^{\pi/2} \phi_p(x)x^2\phi_q(x)dx\right]\left[\int_{-\pi/2}^{\pi/2} \phi_q(x')x^2\phi_p(x')dx'\right] \\
&= \sum_q \left[\int_{-\pi/2}^{\pi/2} \phi_p(u)u^2\phi_q(u)du\right]^2,
\end{aligned}
\tag{5}
$$

where u is a dummy variable.

The integrals involved in evaluating eq. (5) are elementary and straightforward. If one chooses p to be one of the odd states m above, only odd states will contribute to the sum q and one obtains:

$$\left(\frac{\pi^4}{80} - \frac{\left(\frac{(m\pi)^2}{2} - 3\right)}{2m^4}\right) = \sum{}'_{m'=2,4,\ldots} \frac{64m^2m'^2}{(m'^2 - m^2)^4} + \left(\frac{\pi^2}{12} - \frac{1}{2m^2}\right)^2, \tag{6}$$

where $m = 2,\ 4, \ldots$, and the prime in the sum implies, as per the usual convention, that the term $m' = m$ is excluded. Reordering eq. (6), and defining $M = m/2,\ M' = m'/2$, leads to:

$$\sum{}'_{M'=1,2,\ldots} \frac{M'^2}{(M'^2 - M^2)^4} = \frac{\left(4(M\pi)^2 - 15\right)^2}{2^8 3^2 5 M^6}, \tag{7}$$

where $M = 1,\ 2,\ 3\ldots$, an expression not cited in the literature [3, 4, 5]. The l.h.s. of this expression can be written:

$$\sum{}'_{M'=1,2,\ldots} \frac{M'^2}{(M'^2 - M^2)^4} = \sum{}'_{M'=1,2,\ldots} \frac{1}{(M'^2 - M^2)^3} + M^2 \sum{}'_{M'=1,2,\ldots} \frac{1}{(M'^2 - M^2)^4}, \tag{8}$$

which implies that if one knows the expression for $\sum{}'_{M'=1,2,\ldots} \frac{1}{(M'^2 - M^2)^3}$, one can obtain the higher order expression $\sum{}'_{M'=1,2,\ldots} \frac{1}{(M'^2 - M^2)^4}$ with the help of eq. (7).

In the literature one finds the expressions [3, 4, 5]

$$\sum{}'_{M'=1,2\ldots} \frac{1}{(M'^2 - M^2)^1} = \frac{3}{4M^2} \tag{9}$$

$$\sum{}'_{M'=2,3,\ldots} \frac{1}{(M'^2 - 1)^2} = \frac{\pi^2}{12} - \frac{11}{16}. \tag{10}$$

Equation (10) can be generalized by noting that in the higher order expression (7), the product $M\pi$ appears in an even combination. In this way one obtains the new, more general result:

$$\sum{}'_{M'=1,2,\ldots} \frac{1}{(M'^2 - M^2)^2} = \frac{\frac{(M\pi)^2}{12} - \frac{11}{16}}{M^4}. \tag{11}$$

With further effort, and noting that the results of the summations above are even in $M\pi$, one can obtain the next higher-order result:

$$\sum{}'_{M'=1,2,\ldots} \frac{1}{(M'^2 - M^2)^3} = \frac{\frac{-(M\pi)^2}{16} + \frac{21}{32}}{M^6}. \tag{12}$$

One can now carry out the manipulations indicated in eq. (8), with the help of eqs. (7) and (12), and obtain:

$$\sum{}'_{M'=1,2,\ldots} \frac{1}{(M'^2 - M^2)^4} = \frac{16(M\pi)^4 + 600(M\pi)^2 - 7335}{2^8 3^2 5 M^8}. \tag{13}$$

Thus, one has the four, successively higher-order series $\sum{}'_{M'=1,2,\ldots} \frac{1}{(M'^2 - M^2)^p}$, $p = 1,\ 2,\ 3,\ 4$, given by eqs. (9), (11), (12) and (13), of which only the first, i.e. eq. (9), is a standard result. For $p = 2$, eq. (11) is listed in the literature only for the special case $M = 1$, while the series of eq. (7) can be deduced from the new eqs. (12) and (13).

II. Case $\hat{A},\ \hat{B} = |x|$.

If $\hat{A},\ \hat{B} = |x|$, the resulting integrals are again straightforward and, as before, basis states of different parities do not mix. One has in this case:

$$\int_{-\pi/2}^{\pi/2} \phi_p(x) x^2 \phi_p(x) dx = \sum_q \left[\int_{-\pi/2}^{\pi/2} \phi_p(u)|u|\phi_q(u) du \right]^2 . \tag{14}$$

If one chooses p to be one of the odd states m above, only odd states will contribute to the sum q, and one obtains:

$$\frac{\pi^2}{12} - \frac{1}{2m^2} = \sum{}'_{m'=2,4,\ldots} \frac{64((-1)^{m'/2} - (-1)^{m/2})^2 m^2 m'^2}{(m'^2 - m^2)^4 \pi^2} + \left(\frac{\pi}{4}\right)^2 \tag{15}$$

where $m = 2,\ 4, \ldots$, and the prime in the sum again implies that the term $m' = m$ is excluded. Reordering eq. (15), and defining $M = m/2,\ M' = m'/2$, leads to:

$$\sum{}'_{M'=1,2,\ldots} \frac{(1 - (-1)^{M-M'}) M'^2}{(M'^2 - M^2)^4} = \frac{(M\pi)^2 \left((M\pi)^2 - 6\right)}{2^7 3 M^6}, \tag{16}$$

where $M = 1,\ 2,\ 3 \ldots$.

Combining eq. (16) with eq. (7) yields:

$$\sum{}'_{M'=1,2,\ldots} \frac{(-1)^{M'} M'^2}{(M'^2 - M^2)^4} = (-1)^M \frac{\left(1800 + 480(M\pi)^2 - 112(M\pi)^4\right)}{2^{11} 3^2 5 M^6}, \tag{17}$$

where $M = 1,\ 2,\ 3, \ldots$, an expression not cited in the literature [3, 4, 5].

One can now proceed similarly to Section II, with

$$\sum{}'_{M'=1,2,\ldots} \frac{(-1)^{M'} M'^2}{(M'^2 - M^2)^4} = \sum{}'_{M'=1,2,\ldots} \frac{(-1)^{M'}}{(M'^2 - M^2)^3} + M^2 \sum{}'_{M'=1,2,\ldots} \frac{(-1)^{M'}}{(M'^2 - M^2)^4}, \tag{18}$$

which implies that if one knows the expression for $\sum{}'_{M'=1,2,\ldots} \frac{(-1)^{M'}}{(M'^2 - M^2)^3}$, one can obtain the higher order expression $\sum{}'_{M'=1,2,\ldots} \frac{(-1)^{M'}}{(M'^2 - M^2)^4}$ with the help of eq. (17).

In the literature one finds the expressions [3, 4, 5]

$$\sum{}'_{M'=1,2,\ldots} \frac{(-1)^{M'}}{(M'^2 - M^2)^1} = \frac{2 + (-1)^M}{4M^2} \tag{19}$$

$$\sum{}'_{M'=2,3,\ldots} \frac{(-1)^{M'}}{(M'^2 - 1)^2} = \frac{\pi^2}{24} - \frac{5}{16}. \tag{20}$$

Equation (20) can be generalized by noting that in the higher order eq. (16) $M\pi$ appears in an even combination. In this way one obtains the new, more general result:

$$\sum{}'_{M'=1,2,\ldots} \frac{(-1)^{M'}}{(M'^2 - M^2)^2} = (-1)^{M+1} \frac{\left(\frac{(M\pi)^2}{24} + \frac{3}{16} + \frac{(-1)^M}{2}\right)}{M^4}. \tag{21}$$

With further effort, and noting that the results of the summations above are even in $M\pi$, one can obtain the next higher order result:

$$\sum{}'_{M'=1,2,\ldots} \frac{(-1)^{M'}}{(M'^2 - M^2)^3} = (-1)^{M+1} \frac{\left(-\frac{(M\pi)^2}{32} - \frac{5}{32} - \frac{(-1)^M}{2}\right)}{M^6}. \tag{22}$$

One can now carry out the manipulations indicated in eq. (18), with the help of eqs. (17) and (22), one obtains finally:

$$\sum{}'_{M'=1,2,\ldots}\frac{(-1)^{M'}}{(M'^2-M^2)^4}=(-1)^{M+1}\frac{\left(14(M\pi)^4+300(M\pi)^2+1575+(-1)^M5760\right)}{2^8 3^2 5 M^8}. \tag{23}$$

Thus, one has the four successively higher order series $\sum{}'_{M'=1,2,\ldots}\frac{(-1)^{M'}}{(M'^2-M^2)^p}$, $p=1,\ 2,\ 3,\ 4$, given by eqs (19), (21), (22) and (23), of which only the first, i.e. eq. (19), is a standard result. For $p=2$, eq. (21) is listed in the literature [3, 4, 5] only for the special case $M=1$, while the series eq. (17) can be deduced from eqs. (22) and (23).

2. Discussion

The convergence of the series above may be verified using the ratio test [6].

Consider the sum

$$\sum{}'_{M'=1,2,\ldots}\frac{1}{(M'^2-M^2)^p}.$$

The ratio

$$\frac{c_{M'+1}}{c_{M'}}=\frac{\left(M'^2-M^2\right)^p}{\left((M'+1)^2-M^2\right)^p}\sim 1-\frac{2p}{M'},$$

converges provided $2p>0$.

An interesting property of all these series is that they are even in M' and M. Thus

$$\sum{}'_{M'=\ldots,-2,-1,0,1,2,\ldots}\frac{1}{(M'^2-M^2)^p}=2\sum{}'_{M'=1,2,\ldots}\frac{1}{(M'^2-M^2)^p}+\frac{1}{M^{2p}},$$

if for the first term the $'$ implies $|M'|\neq|M|$.

The remainder beyond some M'_{max} is approximately

$$\int_{M'_{\text{max}}}^{\infty}\frac{1}{M'^{2p}}dM'=\frac{1}{(2p-1)M'^{2p-1}_{\text{max}}},$$

a remainder which decreases as p increases.

Since the monotonic series in Section II converge, the alternating series of Section III, definitely converge.

Inspection of the above expressions strongly suggests that for any arbitrary integer p,

$$\sum{}'_{M'=1,2,\ldots}\frac{1}{(M'^2-M^2)^p}=\frac{f\left((M\pi)^2\right)}{M^{2p}},$$

i.e.

$$\sum{}'_{M'=1,2,\ldots}\frac{1}{\left(\left(\frac{M'}{M}\right)^2-1\right)^p}=f\left((M\pi)^2\right),$$

where f is a polynomial in $(M\pi)^2$, while

$$\sum{}'_{M'=1,2,\ldots}\frac{(-1)^{M'}}{(M'^2-M^2)^p}=\frac{g\left((M\pi)^2\right)}{M^{2p}},$$

i.e.

$$\sum{}'_{M'=1,2,\ldots}\frac{(-1)^{M'}}{\left(\left(\frac{M'}{M}\right)^2-1\right)^p}=g\left((M\pi)^2\right),$$

where g is a polynomial in $(M\pi)^2$.

3. Conclusions

By using the standard closure expression, and a particular discrete set of states, one obtains interesting new mathematical summation expressions. In particular one obtains the new results $\sum'_{M'=1,2,\ldots} \frac{1}{(M'^2-M^2)^p}$, $p = 2,\ 3,\ 4$, using the operator x^2, and $\sum'_{M'=1,2,\ldots} \frac{(-1)^{M'}}{(M'^2-M^2)^p}$, $p = 2,\ 3,\ 4$, using the operator $|x|$ in the closure expression and an infinite square well basis. For $p = 1$ these expressions are given in the literature, and for $p = 2$ they are given for the special case $M = 1$. The new numerical (in the sense they involve only integers) summation results of this paper are eqs. (11), (12), (13) and eqs. (21), (22), (23). The same method may be used to obtain other new, higher order and other interesting mathematical series expressions.

Acknowledgments

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