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Off-diagonal Matrix Elements and Sum Rules involving Coulomb and Isotropic Oscillator Functions

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Abstract

Off-diagonal matrix elements and sum rules for the Coulomb and isotropic oscillator systems are obtained from a study of relations between the off-diagonal matrix elements of a general recursion relation.

Key Words: recursion relations, off-diagonal matrix elements, sum rules, Coulomb system, isotropic oscillator system

1. Introduction

In a recent paper [1], a general matrix element recursion relation was obtained without recourse to specific properties of the eigenstates (i.e. the Hamiltonian) involved. This result is as follows:

$$\frac{k(k^2-(2l+1)^2)}{2(k+1)} < ml|r^{k-2}|nl > -\frac{2(p+2k+2)M}{(k+1)\hbar^2} < ml|r^k V(r)|nl >$$
$$+\frac{2M\,(E_{nl}+E_{ml})}{\hbar^2} < ml|r^k|nl > +\frac{2M^2(E_{ml}-E_{nl})^2}{(k+1)(k+2)\hbar^4} < ml|r^{k+2}|nl >= 0, \qquad (1)$$

where given a general Hamiltonian H of the form $H = T + Ar^p$, $H|sl >= E_{sl}|sl >$, and the derivation is valid for diagonal as well as off-diagonal matrix elements. Expression (1) is clearly not valid for $k = -1, -2$, for which values one obtains zero denominators. In the present study we use two non-problematic values of k, namely $k = 0, 1$. In the derivation of expression (1) the integration by parts procedure followed assumes that the functions $u_{sl}(r) = rR_{sl}(r)$ vanish at the origin and at infinity. This in turn imposes conditions on $V(r) = Ar^p$. In this paper we study the potentials $p = -1, 2$ and for these two potentials the resulting bound-state functions $u_{sl}(r)$ vanish at both these limits.

2. Sum Rules

We are interested in the off-diagonal matrix elements of Eq. (1). The diagonal matrix elements for the Coulomb (Kramers' relations) potential ($p = -1$), the isotropic oscillator ($p = 2$), and the bouncer problem ($p = 1$), all of which can be solved analytically, have already been extensively discussed in the literature [2-5]. The off-diagonal matrix elements for the bouncer have also been reported [5]. We therefore concentrate in this note on the Coulomb and isotropic oscillator off-diagonal matrix elements.

If $k = 0$ Eq. (1) reduces, for $m \neq n$, to

$$< ml|V(r)|nl >= \frac{M}{\hbar^2} \frac{(E_{nl} - E_{ml})^2 < ml|r^2|nl >}{2(p+2)}. \tag{2}$$

If $k = 1$, one obtains from Eq. (1) that:

$$l(l+1) < ml|r^{-1}|nl >= -\frac{M(p+4)}{\hbar^2} < ml|rV(r)|nl > + \frac{2M}{\hbar^2} (E_{nl} + E_{ml}) < ml|r|nl >$$
$$+ \frac{M^2(E_{ml} - E_{nl})^2}{3\hbar^4} < ml|r^3|nl >= 0. \tag{3}$$

The first of these results is of immediate interest since it involves a two-term relation. Thus, for the Coulomb system with $V(r) = -Ze^2/(4\pi\epsilon_0 r)$, $p = -1$, $|sl>$ the Coulomb basis states, and $E_{nl} = -Z^2\alpha^2 Mc^2/(2n^2)$, Eq. (2) becomes

$$\left\langle ml \left| \frac{1}{r} \right| nl \right\rangle = -\frac{1}{8} \left(\frac{Mc\alpha Z}{\hbar} \right)^3 \left(\frac{1}{n^2} - \frac{1}{m^2} \right)^2 \left\langle ml \left| r^2 \right| nl \right\rangle, \tag{4}$$

where the ratio of the matrix elements

$$\frac{\langle ml \left| \frac{1}{r} \right| nl \rangle}{\langle ml \left| r^2 \right| nl \rangle}$$

is independent of the angular momentum due to the degeneracy of the energy with respect to l.

If one pre-multiplies Eq. (4) by its complex conjugate, this implies that:

$$\sum_{m \neq n} \frac{\left| \langle nl \left| \frac{1}{r} \right| ml \rangle \right|^2}{\left(\frac{1}{n^2} - \frac{1}{m^2} \right)^4} + \int dk \frac{\left| \langle nl \left| \frac{1}{r} \right| k \rangle \right|^2}{\left(\frac{1}{n^2} + \left(\frac{\hbar k}{McZ\alpha} \right)^2 \right)^4}$$
$$= \frac{1}{64} \left(\frac{Mc\alpha Z}{\hbar} \right)^6 \left[\sum_{m \neq n} \left| \langle nl \left| r^2 \right| ml \rangle \right|^2 + \int dk \left| \langle nl \left| r^2 \right| k \rangle \right|^2 \right]$$
$$= \frac{1}{64} \left(\frac{Mc\alpha Z}{\hbar} \right)^6 \left[\langle nl \left| r^4 \right| nl \rangle - \langle nl \left| r^2 \right| nl \rangle^2 \right] = \frac{1}{64} \left(\frac{Mc\alpha Z}{\hbar} \right)^6 \left[(\Delta r^2)^2 \right]. \tag{5}$$

Many other sum rules may be obtained for this system. For instance, if one instead premultiplies Eq. (4) by $\langle nl \left| \frac{1}{r} \right| ml \rangle$, this leads to:

$$\sum_{m \neq n} \frac{\left| \langle nl \left| \frac{1}{r} \right| ml \rangle \right|^2}{\left(\frac{1}{n^2} - \frac{1}{m^2} \right)^2} + \int dk \frac{\left| \langle nl \left| \frac{1}{r} \right| k \rangle \right|^2}{\left(\frac{1}{n^2} + \left(\frac{\hbar k}{McZ\alpha} \right)^2 \right)^2}$$
$$= -\frac{1}{8} \left(\frac{Mc\alpha Z}{\hbar} \right)^3 \left[\sum_{m \neq n} \left\langle nl \left| \frac{1}{r} \right| ml \right\rangle \langle ml \left| r^2 \right| nl \rangle + \int dk \left\langle nl \left| \frac{1}{r} \right| k \right\rangle \langle k \left| r^2 \right| nl \rangle \right]$$
$$= -\frac{1}{8} \left(\frac{Mc\alpha Z}{\hbar} \right)^3 \left[\langle nl \left| r \right| nl \rangle - \left\langle nl \left| \frac{1}{r} \right| nl \right\rangle \langle nl \left| r^2 \right| nl \rangle \right]. \tag{6}$$

For the isotropic oscillator system, the off-diagonal Eq. (2) yields an identity, namely, with $H = T + 1/2M\omega^2 r^2$, $E_{sl} = (2s + l + 3/2)\hbar\omega$, $|sl>$ the isotropic oscillator basis states, and $p = 2$,

$$< ml|\frac{r^2}{2}|nl >= \frac{(m-n)^2}{2} < ml|r^2|nl >, \tag{7}$$

i.e. either $n - m = \pm 1$ or, $< ml|r^2|nl >= 0$.

Eq. (3) is, as mentioned above, more complicated since it generally involves four terms. For both the Coulomb and the isotropic systems it involves only three terms if $n \neq m$ and, for the special case $l = 0$, it reduces to two terms. Thus, for the Coulomb system,

$$\langle m0\,|r|\,n0\rangle = \frac{1}{12}\left(\frac{Mc\alpha Z}{\hbar}\right)^2 \frac{\left(\frac{1}{n^2}-\frac{1}{m^2}\right)^2}{\left(\frac{1}{n^2}+\frac{1}{m^2}\right)} \left\langle m0\left|r^3\right|n0\right\rangle, \tag{8}$$

which again leads to sum rules if one premultiplies by appropriate matrix elements and uses closure.

For the isotropic oscillator, the $k = 1$ expression for $l = 0$ becomes

$$< m0|r|n0 >= \frac{M\omega}{6\hbar}\frac{(3-2m+2n)(3+2m-2n)}{3+2m+2n} < m0|r^3|n0 > . \tag{9}$$

One has only discrete states for this system, so for instance, for $n = 0$ one directly obtains from Eq. (9) the following sum rules:

$$\left\langle 00\left|r^2\right|00\right\rangle = -\frac{3\hbar}{M\omega}\sum_m \frac{\left\langle 00\left|\frac{1}{r}\right|m0\right\rangle\langle m0\,|r|\,00\rangle}{m-\frac{3}{2}}, \tag{10}$$

$$\left\langle 00\left|r^4\right|00\right\rangle = -\frac{3\hbar}{M\omega}\sum_m \frac{\langle 00\,|r|\,m0\rangle\langle m0\,|r|\,00\rangle}{m-\frac{3}{2}}, \tag{11}$$

$$\left\langle 00\left|r^6\right|00\right\rangle = -\frac{3\hbar}{M\omega}\sum_m \frac{\left\langle 00\left|r^3\right|m0\right\rangle\langle m0\,|r|\,00\rangle}{m-\frac{3}{2}}, \tag{12}$$

or generally:

$$\left\langle 00\left|r^{2q+2}\right|00\right\rangle = -\frac{3\hbar}{M\omega}\sum_m \frac{\left\langle 00\left|r^{2q-1}\right|m0\right\rangle\langle m0\,|r|\,00\rangle}{m-\frac{3}{2}}, \tag{13}$$

where $q = 0, 1, 2...$

If one expands both sides of Eqs. (10), (11), (12) they lead to series for π, namely

$$\pi = \frac{16}{3} - \frac{8}{3} + \frac{2}{5} + \frac{1}{21} + \frac{1}{72} + \frac{1}{176} + \cdots \tag{14}$$

$$\pi = \frac{32}{15} + \frac{16}{15} - \frac{4}{75} - \frac{2}{525} - \frac{1}{1260} - \frac{1}{3960} + \cdots \tag{15}$$

$$\pi = \frac{128}{105} + \frac{64}{35} + \frac{16}{175} + \frac{8}{3675} + \frac{1}{3675} + \frac{1}{16170} + \cdots \tag{16}$$

The sums of the first six terms on the right hand side of Eqs. (14), 15), and (16) are respectively 3.1339, 3.1418, and 3.1416 respectively. This indicates that the convergence improves as q increases in Eq. (13).

3. Conclusions

The off-diagonal results discussed in this paper are Eqs. (2) and (3). For the Coulomb system these become Eq. (4) for any l and Eq. (8) for $l = 0$, while for the isotropic oscillator they become Eq. (7) for any l and Eq. (9) for $l = 0$. Illustrative sum rules obtained from these expressions by premultiplying by appropriate matrix elements, and using closure, are Eqs. (5) and (6) and Eqs. (10) - (12).

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