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Diagonal and Off-Diagonal Recursion Relation for the General Potential $V(r) = Ar^p$

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A recursion relation is derived for the potential $V(r) = Ar^p$. Generally, this connects off-diagonal matrix elements of r^{k-2}, r^{k+p}, r^k, and r^{k+2}. The diagonal case is obtained by setting $m = n$ in this relation. The relation is derived by elementary methods and without recourse to specific properties of the eigenstates. Finally, this relation is studied for the familiar potentials $p = -1, 1, 2$.

1. INTRODUCTION

It is useful to have a general recursion relation that one can apply to any radial potential $V(r) = Ar^p$. A *diagonal* recursion relation was obtained many years ago for the Coulomb potential ($p = -1$), the so called Kramers relation (Messiah, 1961). This relation connects the Coulomb-basis diagonal matrix elements $\langle r^N\rangle$, $\langle r^{N-1}\rangle$, and $\langle r^{N-2}\rangle$, and was recently rederived using the Generalized Hellmann–Feynman Theorem (Balasubramanian, 2000). Balasubramanian (2000) also applied the Hellmann–Feynman Theorem to the harmonic oscillator ($p = 2$), for which potential it yields a relation between the oscillator basis diagonal matrix elements $\langle r^{2N+2}\rangle$, $\langle r^{2N}\rangle$, and $\langle r^{2N-2}\rangle$. This relation as well has been known for many years (Beker, 1997).

The usefulness and popularity of recursion relations lies in the fact that they point out to the student that different quantum mechanical matrix elements for a given potential are related. Consequently, one need not go through the tedium of evaluating matrix elements that are in fact interrelated. The student normally first sees this property in the quantum mechanical virial theorem, where the matrix elements of the potential and kinetic energies are seen to be related.

In another recent paper (Goodmanson, 2000), the one-dimensional bouncer ($p = 1$) is examined. By using properties of the Airy functions, Goodmanson (2000) relates z^{p-4}, z^{p-2}, z^{p-1}, and z^p matrix elements for this potential.

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Section 2 of the present paper involves a straightforward derivation for the potential $V(r) = Ar^p$, of a recursion relation that connects *off-diagonal* matrix elements of r^{k-2}, r^{k+p}, r^k, and r^{k+2}. However, it also subsumes diagonal matrix elements as a special case for which diagonal matrix elements (expectation values) of r^{k-2}, r^{k+p}, and r^k are seen to be related. No specific properties of the eigenstates are required in this derivation. Thus, the derivation can easily be followed and reproduced by an advanced undergraduate or graduate student. The derivation being general, one can study the relation obtained for the Coulomb, oscillator, or bouncer, where analytic relations are known. This is done in Sections 3 and 4 of this paper. Additionally, this recursion relation is valid for general potentials $V(r) = Ar^p$, $p \neq -1, 1, 2$, where individual matrix elements must be evaluated numerically.

2. DERIVATION OF THE RECURSION RELATION

The Schrödinger equation for the potential $V(r)$ and radial eigenstates $R_{nl}(r) = u_{nl}(r)/r$, when written in terms of $u_{nl}(r)$ becomes

$$u''_{nl}(r) = \left\{2(V(r) - E_{nl}) + \frac{l(l+1)}{r^2}\right\}u_{nl}(r). \tag{1}$$

Here we have set $m = \hbar = 1$. In what follows the l in $u_{nl}(r)$ is suppressed to make the expressions less cumbersome. The only property used is that $u_{nl}(r) = 0$ for $r = 0, \infty$.

We first consider the integral $\int_0^\infty u_m(r)u_n(r)r^k\,dr$. Integrating by parts,

$$\int_0^\infty u_m(r)u_n(r)r^k\,dr = -\frac{1}{k+1}\int_0^\infty d(u_m(r)u_n(r))r^{k+1}\,dr,$$

i.e.

$$\langle m|r^k|n\rangle = -\frac{1}{k+1}\int_0^\infty (u'_m(r)r^{k+1}u_n(r) + u_m(r)r^{k+1}u'_n(r))\,dr. \tag{2}$$

Similarly, the integral

$$\begin{aligned}\int_0^\infty u'_m(r)u'_n(r)r^k\,dr &= -\frac{1}{k+1}\int_0^\infty d(u'_m(r)u'_n(r))r^{k+1}\,dr\\ &= -\frac{1}{k+1}\int_0^\infty (u'_m(r)r^{k+1}u''_n(r) + u''_m(r)r^{k+1}u'_n(r))\,dr. \end{aligned}\tag{3}$$

However, one can also write this integral as

$$\int_0^\infty u'_m u'_n r^k\, dr = -\frac{1}{2}\left\{\int_0^\infty d(r^k u'_m(r))u_n(r)\, dr + \int_0^\infty d(r^k u'_n(r))\, u_m(r)\, dr\right\}$$
$$= -\frac{k}{2}\int_0^\infty (u'_m r^{k-1} u_n + u_m r^{k-1} u'_n)\, dr$$
$$-\frac{1}{2}\int_0^\infty r^k (u''_m u_n + u_m u''_n)\, dr \tag{4}$$

or, using Eq. (2) with $k \to k-2$,

$$\int_0^\infty u'_m(r) u'_n(r) r^k\, dr = \frac{k(k-1)}{2}\langle m|r^{k-2}|n\rangle - \frac{1}{2}\int_0^\infty r^k (u''_m u_n + u''_n u_m)\, dr. \tag{5}$$

Combining Eqs. (3) and (5) one then has

$$\frac{k(k-1)}{2}\langle m|r^{k-2}|n\rangle = \int_0^\infty \left(\frac{u_m}{2} r^k - \frac{1}{k+1} u'_m r^{k+1}\right) u''_n\, dr$$
$$+ \int_0^\infty \left(\frac{u_n}{2} r^k - \frac{1}{k+1} u'_n r^{k+1}\right) u''_m\, dr. \tag{6}$$

If one substitutes the Schrödinger Eq. (1) for u''_n, and u''_m, in Eq. (6), and assumes the explicit form Ar^p for $V(r)$, one obtains after a little manipulation

$$\frac{k(k^2 - (2l+1)^2)}{2(k+1)}\langle m|r^{k-2}|n\rangle - \frac{2(p+2k+2)}{k+1}$$
$$\times\ \langle m|r^k V(r)|n\rangle + (E_n + E_m)\langle m|r^k|n\rangle - \frac{2}{k+1}$$
$$\times \left[E_n \int_0^\infty u'_m r^{k+1} u_n\, dr + \ E_m \int_0^\infty u_m r^{k+1} u'_n\, dr\right] = 0. \tag{7}$$

This is the desired relation except for the last two terms that involve derivatives. But,

$$\int_0^\infty u'_m r^{k+1} u_n\, dr = -\frac{1}{k+2}\int_0^\infty d(u'_m u_n) r^{k+2}\, dr$$
$$= -\frac{1}{k+2}\int_0^\infty (u''_m u_n + u'_m u'_n)\, r^{k+2}\, dr. \tag{8}$$

Hence

$$E_n \int_0^\infty u_m' r^{k+1} u_n \, dr + E_m \int_0^\infty u_m r^{k+1} u_n' \, dr$$
$$= -\frac{1}{k+2} E_n \int_0^\infty r^{k+2} u_m'' u_n \, dr - \frac{1}{k+2} E_m \int_0^\infty r^{k+2} u_m u_n'' \, dr$$
$$- \frac{E_m + E_n}{k+2} \int_0^\infty u_m' u_n' r^{k+2} \, dr. \tag{9}$$

Using Eq. (5) with $k \to k+2$ in Eq. (9) one then obtains

$$E_n \int_0^\infty u_m' r^{k+1} u_n \, dr + E_m \int_0^\infty u_m r^{k+1} u_n' \, dr$$
$$= -\frac{(E_m + E_n)(k+1)}{2} \langle m|r^k|n\rangle$$
$$+ \frac{(E_m - E_n)}{2(k+2)} \int_0^\infty (u_m'' u_n - u_m u_n'') r^{k+2} \, dr. \tag{10}$$

A final substitution of the Schrödinger Eq. (1) to eliminate u_m'' and u_n'' in Eq. (10), yields the following result:

$$E_n \int_0^\infty u_m' r^{k+1} u_n \, dr + E_m \int_0^\infty u_m r^{k+1} u_n' \, dr$$
$$= -\frac{(E_m + E_n)(k+1)}{2} \langle m|r^k|n\rangle - \frac{(E_m - E_n)^2}{(k+2)} \langle m|r^{k+2}|n\rangle. \tag{11}$$

When Eq. (11) is substituted in Eq. (7) one obtains the desired general result:

$$\frac{k(k^2 - (2l+1)^2)}{2(k+1)} \langle m|r^{k-2}|n\rangle - \frac{2(p + 2k + 2)}{k+1} \langle m|r^k V(r)|n\rangle$$
$$+ 2(E_n + E_m)\langle m|r^k|n\rangle + \frac{2(E_m - E_n)^2}{(k+1)(k+2)} \langle m|r^{k+2}|n\rangle = 0. \tag{12}$$

This expression is not valid if $k = -1$, or -2, as can be seen if one carefully examines the surface terms in this derivation.

3. DIAGONAL CASE

Consider the case $m = n$ in Eq. (12). The last term in then zero and the recursion relation reduces to

$$\frac{k(k^2 - (2l+1)^2)}{2(k+1)} \langle m|r^{k-2}|m\rangle - \frac{2(p + 2k + 2)}{k+1} \langle m|r^k V(r)|m\rangle$$
$$+ 4E_m \langle m|r^k|m\rangle = 0. \tag{13}$$

If additionally $k = 0$, this reduces to the quantum mechanical virial theorem (Merzbacher, 1970):

$$E_m = \frac{p+2}{2} \langle m|V(r)|m\rangle$$

or if T is the kinetic energy operator

$$\langle m|T|n\rangle = \frac{p}{2} \langle m|V(r)|m\rangle. \tag{14}$$

If one substitutes $V(r) = \frac{1}{2}r^2$ and $E_m = (2m + l + \frac{3}{2})$, in Eq. (13), this reduces to the familiar oscillator result (Balasubramanian, 2000; Beker, 1997):

$$\frac{k(k^2 - (2l+1)^2)}{2(k+1)} \langle m|r^{k-2}|m\rangle - \frac{2(k+2)}{k+1} \langle m|r^{k+2}|m\rangle + 4\left(2m + l + \frac{3}{2}\right) \langle m|r^k|m\rangle = 0. \tag{15}$$

For the Coulomb potential $V(r) = -\frac{1}{r}$ and $E_m = -\frac{1}{2m^2}$ one obtains Kramers' relation.

Substituting the potential $V(r) = r$, and with $l = 0$ in Eq. (13), one has the three-dimensional bouncer with zero angular momentum:

$$\frac{k(k-1)}{2} \langle m|r^{k-2}|m\rangle - \frac{2(2k+3)}{k+1} \langle m|r^{k+1}|m\rangle + 4E_m \langle m|r^k|m\rangle = 0. \tag{16}$$

This is equivalent to the diagonal results in Goodmanson (2000) if one bears in mind that Goodmanson's Schrödinger equation is given without the factor 1/2.

4. OFF-DIAGONAL CASE

Consider the case $m \neq n$ and $k = 0$. Then

$$\langle m|V(r)|n\rangle = \frac{(E_n - E_m)^2 \langle m|r^2|n\rangle}{2(p+2)}. \tag{17}$$

If one substitutes $p = 1$ in Eq. (12) one gets the off-diagonal results of Goodmanson (2000) with the same considerations as earlier about the absence of a factor 1/2 in Goodmanson's Schrödinger equation.

Many other results can be obtained from Eq. (12), by choosing $k \neq 0$, and specifying other potentials, etc.

5. CONCLUSIONS

The new result derived in this paper, namely Eq. (12), is a recursion relation for a general potential $V(r) = Ar^p$. It involves a recursion relation for off-diagonal matrix elements if $m \neq n$, and, for the special case $m = n$, for diagonal matrix elements. Several interesting special results follow from this new, general recursion relation.

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