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Group-theoretical derivation of the matrix elements of a momentum-dependent nuclear potential

M J Englefield

Department of Mathematics, Monash University, Clayton, Victoria 3168, Australia

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Abstract. The operators r^2, p^2 and $\boldsymbol{r}.\boldsymbol{p}+\boldsymbol{p}.\boldsymbol{r}$ are a basis of a representation of the algebra $O_{2,1}$. Using harmonic oscillator wavefunctions with a fixed angular momentum as basis of the representation space, the isometrically equivalent representation in work by Barut can be identified. This allows one to write down formulae for matrix elements, relative to oscillator wavefunctions, of any operator of the corresponding group representation. These include $\exp(\mathrm{i}cr^2)$, $\exp(\mathrm{i}q^2p^2/\hbar^2)$, their products, and the scaling operator. One can thus obtain an algebraic derivation of the matrix elements of a momentum-dependent nuclear interaction proposed by Tabakin and Davies.

1. Introduction

Potential representations of the nucleon–nucleon interaction often depend on the relative momentum $\boldsymbol{p}$ of the two particles as well as on their relative position $\boldsymbol{r}$. One such non-local potential, introduced by Tabakin and Davies (1966) to represent the (singlet) interaction, has the form

$$V(r,p) = -V_1\,\mathrm{e}^{-a^2r^2} + C(p)\,\mathrm{e}^{-b^2r^2} + \mathrm{e}^{-b^2r^2}C(p) \tag{1}$$

with

$$C(p) = V_2(p^2/\hbar^2b^2)\exp(-s^2p^2/\hbar^2). \tag{2}$$

(In these equations, all symbols except r and p represent constants.)

In applications, matrix elements of the potential are required, and in particular matrix elements between harmonic oscillator wavefunctions ϕ_{nlm}. Since $C(p)$ acts as a differential operator on wavefunctions of position, the usual straightforward integration formulae are not available. However, Tabakin and Davies devised Laplace transform methods to evaluate $C(p)\phi_{nlm}$ and then the matrix elements of the potential. Their formulae were later used by Pearson and Saunier (1968), and Fu and Yost (1970). Tabakin and Davies noted that the effect of $C(p)$ on ϕ_{nlm} was like that of a scaling operator.

This paper presents an algebraic derivation of these matrix elements, using group theory. The operators r^2, p^2, and $(\boldsymbol{r}.\boldsymbol{p}+\boldsymbol{p}.\boldsymbol{r})$ are a basis of a representation of the Lie algebra $O_{2,1}$. This representation includes the oscillator Hamiltonian. The algebra generates a non-compact group, and the corresponding group representation includes operators of the form $\exp(\mathrm{i}\mu r^2)$ and $\exp(\mathrm{i}\nu p^2)$, and their products (in either order). Matrix elements of these operators, for real μ and ν, can therefore be written down from group-theoretical results obtained by Barut (1967). The formulae thus obtained remain valid when $\mathrm{i}b^2$ and $\mathrm{i}s^2/\hbar^2$ are substituted for μ and ν, giving the required matrix elements.

Barut uses an equivalent representation in the space of monomials of two complex variables: the elements of the algebra are represented by differential operators, and the elements of the group are represented by linear transformations of type SU(1, 1). This method is therefore rather similar to the conventional (see, for example, Wigner 1959) derivation of the matrix elements of rotations using an equivalent representation on polynomials in two complex variables.

2. Representations of $O_{2,1}$

The relevant representation of the algebra $O_{2,1}$ was given by Goshen and Lipkin (1959). For the present application this section will describe (with some slight changes in notation) results given by Haskell and Wybourne (1972).

Let

$$\begin{aligned} X &= (p^2/4\beta^2\hbar^2)-(\beta^2r^2/4) \\ Y &= (\boldsymbol{r}.\boldsymbol{p}+\boldsymbol{p}.\boldsymbol{r})/4\hbar \\ Z &= (p^2/4\beta^2\hbar^2)+(\beta^2r^2/4). \end{aligned} \tag{3}$$

Then

$$XY-YX=-\mathrm{i}Z \qquad YZ-ZY=\mathrm{i}X \qquad ZX-XZ=\mathrm{i}Y, \tag{4}$$

which are the standard commutation relations for a basis of a representation of $O_{2,1}$. This is true for any value of the constant β, but for the present objective of obtaining matrix elements relative to oscillator wavefunctions, β will be the usual oscillator constant: for an oscillator of frequency ω and mass M, $\beta^2=M\omega/\hbar$, and then $2\hbar\omega Z$ is the oscillator Hamiltonian. (Tabakin and Davies have $M=\frac{1}{2}m$, which is the reduced mass for the relative motion of nucleons of mass m.)

Since X, Y and Z are scalars, they operate on angular momentum eigenstates without changing the angular momentum quantum numbers l and m. For each fixed value of (l, m), an irreducible representation of $O_{2,1}$ is obtained with X, Y and Z acting in the representation space consisting of the set of wavefunctions having this angular momentum. To get the required matrix elements, the oscillator wavefunctions ϕ_{nlm} are used as a basis of this representation space. These functions will be written ϕ_n subsequently.

The energy eigenvalue is $(2n+l+\frac{3}{2})\hbar\omega$, so that

$$Z\phi_n=(n+\tfrac{1}{2}l+\tfrac{3}{4})\phi_n. \tag{5}$$

By writing

$$X\pm\mathrm{i}Y=Z-\tfrac{1}{2}\beta^2r^2\pm\tfrac{3}{4}\pm\tfrac{1}{2}r\frac{\partial}{\partial r},$$

using the explicit expression for ϕ_n given by Tabakin and Davies, and using properties of the Laguerre polynomials, one obtains

$$(X-\mathrm{i}Y)\phi_n=\surd[n(n+l+\tfrac{1}{2})]\phi_{n-1} \tag{6}$$

$$(X+\mathrm{i}Y)\phi_n=\surd[(n+1)(n+l+\tfrac{3}{2})]\phi_{n+1}. \tag{7}$$

Equations (5), (6) and (7) could be deduced from (4) by a completely algebraic argument (Goshen and Lipkin 1959). This would be almost the same as deriving from angular momentum commutation rules the angular momentum eigenvalues and the action of the shift operators. However, in order to get the results of Tabakin and Davies, states with the same phase factors must be used, and the only way to ensure this is to evaluate $(X\pm \mathrm{i}Y)\phi_n$ with explicit wavefunctions ϕ_n and the differential operator representation of $X\pm\mathrm{i}Y$.

The main difference between angular momentum theory and the results given in equations (4)–(7) is as follows. In angular momentum theory, for a given value of l (i.e. eigenvalue of L^2), there are just $(2l+1)$ eigenvalues m of L_z $(m=-l, -l+1, \ldots, +l)$ and the shift operators $L_x\pm\mathrm{i}L_y$ give zero when $m=\pm l$. In the $O_{2,1}$ representations, for a given l the eigenvalues of Z have a lower bound $\frac{1}{2}l+\frac{3}{4}$, and applying the lowering operator $X-\mathrm{i}Y$ to the eigenfunction ϕ_0 gives zero. This is seen by putting $n=0$ in (5) and (6). However, the raising operator always gives a new eigenfunction ($n=0$, 1, 2, ...), since the coefficient on the right-hand side of (7) cannot vanish. Thus the irreducible representation is infinite dimensional.

It is now easy to identify these representations of $O_{2,1}$ in terms of the classification given by Barut (1967). His operator L_{12} corresponds to Z, so the representation is type $\mathscr{D}^+(\phi)$ in which L_{12} has a minimum eigenvalue $-\phi$, and the Casimir operator has the eigenvalue $-\phi(\phi+1)$. Here $\phi=-\frac{1}{2}l-\frac{3}{4}$, and the eigenvalue of the Casimir operator $X^2+Y^2-Z^2$ is $-\frac{1}{4}(l^2+l-\frac{3}{4})$. This may be checked by writing the Casimir operator in the form $(X-Z)(X+Z)+\mathrm{i}Y+Y^2$, and substituting (3), and using the equations

$$\mathrm{i}Y=\frac{1}{2}r\frac{\partial}{\partial r}+\frac{3}{4}, \qquad \frac{r^2p^2}{\hbar^2}=-r^2\frac{\partial^2}{\partial r^2}-2r\frac{\partial}{\partial r}+\frac{L^2}{\hbar^2}.$$

The correspondence between (3) and the fundamental 2×2 matrix representation of $O_{2,1}$ is (using the Pauli spin matrices)

$$X\leftrightarrow\tfrac{1}{2}\mathrm{i}\sigma_x, \qquad Y\leftrightarrow\tfrac{1}{2}\mathrm{i}\sigma_y, \qquad Z\leftrightarrow\tfrac{1}{2}\sigma_z. \tag{8}$$

3. The group representations

The operators $\mathrm{e}^{\mathrm{i}A}$, where A are the operators of a Hermitian representation of $O_{2,1}$, give a unitary representation of a corresponding group. The representation space will be the same, and the work of Barut (1967) allows one to write down the matrix elements $\langle\phi_n|\mathrm{e}^{\mathrm{i}A}|\phi_{n'}\rangle$ relative to the states ϕ_n.

From (1) and (2), the matrix elements of $V(r,p)$ can then be obtained by choosing for A

$$c\beta^2r^2=2c(Z-X) \tag{9}$$

or

$$qp^2/\hbar^2=2\beta^2q(Z+X) \tag{10}$$

(in which c and q are numbers).

The case

$$A=2Y\ln\lambda \tag{11}$$

is also of interest, because $2\mathrm{i}Y=\frac{3}{2}+r(\partial/\partial r)=\frac{3}{2}+\boldsymbol{r}.\boldsymbol{\nabla}$, and $\exp(2\mathrm{i}Y\ln\lambda)$ is the scaling operator with the property (Pratt and Jordan 1966)

$$\exp(2\mathrm{i}Y\ln\lambda)\psi(r)=(\sqrt{\lambda})^3\psi(\lambda r). \tag{12}$$

(The factor $(\sqrt{\lambda})^3$ preserves the normalization of ψ.)

The correspondence (8) gives $2\mathrm{i}Y\ln\lambda\leftrightarrow-\sigma_y\ln\lambda$. Then the matrix $\exp(-\sigma_y\ln\lambda)$, which can be evaluated using the exponential series, is the matrix corresponding to the scaling operator in the fundamental 2×2 representation of the group:

$$\exp(2\mathrm{i}Y\ln\lambda)\to\exp(-\sigma_y\ln\lambda)=\frac{1}{2}\begin{bmatrix}\lambda+1/\lambda & \mathrm{i}\lambda-\mathrm{i}/\lambda\\ -\mathrm{i}\lambda+\mathrm{i}/\lambda & \lambda+1/\lambda\end{bmatrix}. \tag{13}$$

Similarly,

$$\exp(\mathrm{i}c\beta^2r^2)\to\begin{bmatrix}1+\mathrm{i}c & c\\ c & 1-\mathrm{i}c\end{bmatrix} \tag{14}$$

$$\exp\left(\frac{\mathrm{i}qp^2}{\hbar^2}\right)\to\begin{bmatrix}1+\mathrm{i}\beta^2q & -\beta^2q\\ -\beta^2q & 1-\mathrm{i}\beta^2q\end{bmatrix}. \tag{15}$$

The matrices corresponding to $\exp(\mathrm{i}c\beta^2r^2)\exp(\mathrm{i}qp^2/\hbar^2)$ or $\exp(\mathrm{i}qp^2/\hbar^2)\exp(\mathrm{i}c\beta^2r^2)$ may now be obtained by taking products of the matrices (14) and (15) in the appropriate order.

Taking the exponential function of a matrix belonging to the fundamental representation of the algebra (i.e. a real linear combination of the matrices in (8)) always gives a matrix of the form

$$W=\begin{bmatrix}\xi & \eta\\ \bar{\eta} & \bar{\xi}\end{bmatrix} \tag{16}$$

for some complex numbers ξ and η, with $|W|=1$. The representation used by Barut (1967) to evaluate matrix elements consists of the corresponding linear transformations of two complex variables z and w, acting on monomial functions $z^nw^{2\phi-n}$, i.e. the transformations

$$z^nw^{2\phi-n}\to(\xi z+\bar{\eta}w)^n(\eta z+\bar{\xi}w)^{2\phi-n}.$$

After defining an inner product by

$$\langle z^nw^{2\phi-n}|z^{n'}w^{2\phi-n'}\rangle=\delta_{n,n'}n!/(-2\phi)(1-2\phi)\ldots(n-1-2\phi), \tag{17}$$

matrix elements are obtained by using the binomial expansion. Phase and normalization factors must be chosen so that the representation is isometrically equivalent to the one defined on the oscillator wavefunctions, i.e. inner products (matrix elements) are preserved. The required correspondence between representation spaces is

$$\phi_n\leftrightarrow|n\rangle=\binom{n-2\phi-1}{n}^{1/2}z^n(\mathrm{i}w)^{2\phi-n}. \tag{18}$$

The correspondence between representations of the algebra is given by

$$Z\leftrightarrow\frac{1}{2}z\frac{\partial}{\partial z}-\frac{1}{2}w\frac{\partial}{\partial w},\qquad X+\mathrm{i}Y\leftrightarrow\mathrm{i}z\frac{\partial}{\partial w},\qquad X-\mathrm{i}Y\leftrightarrow\mathrm{i}w\frac{\partial}{\partial z}.$$

The definition (17) ensures that the operators corresponding to X, Y and Z are Hermitian, and the phase factor $\mathrm{i}^{2\phi-n}$ in (18) ensures that the equations

$$\left(\mathrm{i}w\frac{\partial}{\partial z}\right)|n\rangle = \sqrt{[n(n-1-2\phi)]}|n-1\rangle$$

$$\left(\mathrm{i}z\frac{\partial}{\partial w}\right)|n\rangle = \sqrt{[(n+1)(n-2\phi)]}|n+1\rangle$$

have exactly the same constant factors as (6) and (7). It is then true that

$$\langle n|W|n'\rangle = \langle\phi_n|\mathrm{e}^{\mathrm{i}A}|\phi_{n'}\rangle$$

when $\mathrm{e}^{\mathrm{i}A} \to W$.

Putting in these phase and normalization factors, the matrix element of the transformation defined by the matrix (16) is (Barut 1967):

$$\langle n|W|n'\rangle = \frac{\Gamma(n+n'+l+\frac{3}{2})(-\mathrm{i}\eta)^n(-\mathrm{i}\bar{\eta})^{n'}{}_2F_1}{[n!n'!\Gamma(n+l+\frac{3}{2})\Gamma(n'+l+\frac{3}{2})]^{1/2}\bar{\xi}^{n+n'+l+\frac{3}{2}}}$$

where ${}_2F_1$ is the Gauss hypergeometric function

$${}_2F_1(-n, -n'; -n-n'-l-\tfrac{1}{2}; \xi\bar{\xi}/\eta\bar{\eta}).$$

In terms of the normalization factor N_{nl} used by Tabakin and Davies (1966), this result may be written

$$\langle n|W|n'\rangle = \frac{N_{nl}N_{n'l}\Gamma(n+n'+l+\frac{3}{2})(-\mathrm{i}\eta)^n(-\mathrm{i}\bar{\eta})^{n'}{}_2F_1}{2\beta^3 n!n'!\bar{\xi}^{n+n'+l+\frac{3}{2}}}. \tag{19}$$

4. Potential matrix elements

To obtain the required matrix elements, it is now only necessary to compare (14) and (15) with (16) to get ξ and η, and then substitute into (19).

(i) From (14) and (16), the transformation corresponding to $\exp(\mathrm{i}c\beta^2r^2)$ has $\xi = 1+\mathrm{i}c$, $\bar{\xi} = 1-\mathrm{i}c$, and $\eta = \bar{\eta} = c$. With these substitutions, (19) will give $\langle\phi_n|\exp(\mathrm{i}c\beta^2r^2)|\phi_{n'}\rangle$. The matrix elements of $V_1\exp(-a^2r^2)$ may then be obtained by putting $c = \mathrm{i}a^2/\beta^2$, and multiplying by V_1. Evidently the result may be obtained from (19) by replacing ξ by $1-a^2/\beta^2$, $\bar{\xi}$ by $1+a^2/\beta^2$, η and $\bar{\eta}$ by $\mathrm{i}a^2/\beta^2$. Thus

$$\langle\phi_n|V_1\exp(-a^2r^2)|\phi_{n'}\rangle = \frac{V_1N_{nl}N_{n'l}\Gamma(n+n'+l+\frac{3}{2})a^{2n+2n'}\beta^{2l}{}_2F_1}{2n!n'!(\beta^2+a^2)^{n+n'+l+\frac{3}{2}}} \tag{20}$$

with

$${}_2F_1 = {}_2F_1(-n, -n'; -n-n'-l-\tfrac{1}{2}; 1-\beta^4/a^4).$$

(ii) Multiplying the matrices in (14) and (15) shows that the transformation corresponding to $\exp(\mathrm{i}qp^2/\hbar^2)\exp(\mathrm{i}c\beta^2r^2)$ has $\xi = 1+\mathrm{i}c+\mathrm{i}\beta^2q-2c\beta^2q$ and $\eta = c-\beta^2q+2\mathrm{i}c\beta^2q$. The matrix elements of $\exp(-s^2p^2/\hbar^2)\exp(-b^2r^2)$ are therefore obtained from (19) by the following replacements:

ξ by $\quad 1-(b^2/\beta^2)-\beta^2s^2+2b^2s^2 = (2-t)(1+U-V)$

$\bar{\xi}$ by $\quad 1+(b^2/\beta^2)+\beta^2s^2+2b^2s^2 = tV$

η by $\quad ib^2/\beta^2 - is^2\beta^2 - 2ib^2s^2 = i(2-t)(V-U)$

$\bar{\eta}$ by $\quad ib^2/\beta^2 - is^2\beta^2 + 2ib^2s^2 = it(V-1)$

where $t = 1 + 2s^2\beta^2$, $U = (1/2t) + 1/2(2-t)$ and $V = \frac{1}{2} + (1/2t) + (b/\beta)^2$ are quantities used by Tabakin and Davies (1966) in their formulae for the matrix elements. The argument $(\xi\bar{\xi}/\eta\bar{\eta})$ of the hypergeometric function in (19) becomes

$$x = (V-U-1)V/(V-U)(V-1).$$

The result is

$$\frac{\langle\phi_n|\exp(-s^2p^2/\hbar^2)\exp(-b^2r^2)|\phi_{n'}\rangle}{N_{nl}N_{n'l}\Gamma(n+n'+l+\frac{3}{2})} = \frac{(2-t)^n(V-U)^n(1-1/V)^{n'}{}_2F_1(-n, -n'; -n-n'-l-\frac{1}{2}; x)}{2\beta^3 n!\,n'!\,(tV)^{n+l+\frac{3}{2}}}. \tag{21}$$

Interchanging n and n' gives $\langle\phi_n|\exp(-b^2r^2)\exp(-s^2p^2/\hbar^2)|\phi_{n'}\rangle$.

(iii) The matrix elements $\langle n|p^2|n''\rangle$ are well known (or may be deduced from the correspondence (8)). They are non-zero only for $n'' = n$, $n \pm 1$, allowing the matrix elements of $C(p)\exp(-b^2r^2)$ to be written as a sum of three terms using (21):

$$\begin{aligned}
&\frac{2b^2\beta n!\,n'!\,(tV)^{n+l+\frac{3}{2}}}{V_2(1-1/V)^{n'}(2-t)^n(V-U)^nN_{nl}N_{n'l}}\langle\phi_n|C(p)\exp(-b^2r^2)|\phi_{n'}\rangle \\
&\quad = \frac{n(n+l+\frac{1}{2})tV\Gamma(n+n'+l+\frac{1}{2})}{(2-t)(V-U)}{}_2F_1(-n+1, -n'; -n-n'-l+\frac{1}{2}; x) \\
&\qquad + (2n+l+\tfrac{3}{2})\Gamma(n+n'+l+\tfrac{3}{2}){}_2F_1(-n, -n'; -n-n'-l-\tfrac{1}{2}; x) \\
&\qquad + \frac{(2-t)(V-U)}{Vt}\Gamma(n+n'+l+\tfrac{5}{2}){}_2F_1(-n-1, -n'; -n-n'-l-\tfrac{3}{2}; x).
\end{aligned} \tag{22}$$

Again interchanging n and n' gives $\langle\phi_n|\exp(-b^2r^2)C(p)|\phi_{n'}\rangle$.

(iv) Putting

$${}_2F_1(-n, -n'; -n-n'-u+1; x) = \frac{n!\,n'!}{\Gamma(n+n'+u)}\sum_{k=0}^{\min(n,n')}\frac{\Gamma(n+n'+u-k)(-x)^k}{k!(n-k)!(n'-k)!} \tag{23}$$

into (20), with $u = l + \frac{3}{2}$, immediately gives part of the formula of Tabakin and Davies (1966). The rest of their result may be obtained from (22) after some algebra which commences as follows: use (23) in the first term with $u = l + \frac{1}{2}$ and v as the summation variable, take $n + l + \frac{1}{2}$ inside the summation and write it as $(n + n' + l + \frac{1}{2} - v) - (n' - v)$, thus obtaining two terms; use (23) in the third term with $u = l + \frac{5}{2}$ and j as the summation variable, take $n + 1$ (from $(n+1)!$) inside the summation and write it as $(n + 1 - j) + j$ to obtain two terms.

Some of this algebra is equivalent to using the relations between contiguous hypergeometric functions. The formulae (21) and (22) may be put in alternative forms using transformation formulae to convert to hypergeometric functions of $1/x$ or $(1-x)$. A different form may be advantageous for numerical calculations.

The equivalence of (20) and (22) to the results of Tabakin and Davies shows that the replacements of c by ia^2/β^2 and q by is^2 are valid, although it is clear that this can only be done after using the group-theoretical result (19).

5. The scaling operator

The Tabakin and Davies formula for $C(p)\phi_n$ is equivalent to

$$\exp(-s^2p^2/\hbar^2)\phi_n = (t\sqrt{U})^{-2n-l-\frac{3}{2}} \exp(s^2\beta^4Ur^2) \exp(2\mathrm{i}Y \ln\sqrt{U})\phi_n \tag{24}$$

in which $\exp(2\mathrm{i}Y\ln\sqrt{U})$ is a scaling operator as in (12). To establish (24) it is sufficient to show that the operators

$$(t\sqrt{U})^{2n+l+\frac{3}{2}} \exp(-s^2\beta^4Ur^2) \exp(-s^2p^2/\hbar^2) \tag{25}$$

and $\exp(2\mathrm{i}Y\ln\sqrt{U})$ have the same matrix elements.

From (13), the matrix elements of the scaling operator are given by (19) with $\xi = \frac{1}{2}(U+1)/\sqrt{U}$ and $\eta = \frac{1}{2}\mathrm{i}(U-1)/\sqrt{U}$, i.e.

$$\langle\phi_n|\exp(2\mathrm{i}Y\ln\sqrt{U})|\phi_{n'}\rangle = \frac{(-1)^{n'}\Gamma(n+n'+l+\frac{3}{2})N_{nl}N_{n'l}}{2\beta^3 n!n'!}\left(\frac{U-1}{U+1}\right)^{n+n'}\left(\frac{2\sqrt{U}}{U+1}\right)^{l+\frac{3}{2}} {}_2F_1 \tag{26}$$

in which the argument of the hypergeometric function is $(U+1)^2/(U-1)^2$.

The matrix elements of (25) may be obtained from (21) by interchanging n and n', replacing b^2 by $s^2\beta^4U$, and multiplying by $(t\sqrt{U})^{2n+l+\frac{3}{2}}$. The result is just (26), because with this choice of b^2, V is replaced by $\frac{1}{2}+\frac{1}{2}U$.

The matrix element (26) is the same as the overlap integral between oscillator wavefunctions with different spring constants β and $\beta\sqrt{U}$. Using the hypergeometric transformation formula ($n \geqslant n'$)

$$\begin{aligned}&{}_2F_1(-n,-n';-n-n'-l-\tfrac{1}{2};x)\\ &\quad=\frac{\Gamma(n+l+\frac{3}{2})(1-x)^{n'}n!}{\Gamma(n+n'+l+\frac{3}{2})(n-n')!}{}_2F_1(-n',-n'-l-\tfrac{1}{2};n-n'+1;1/(1-x)),\end{aligned}$$

and putting $\sqrt{U}=\alpha$ so that $x=(1+\alpha^2)^2/(1-\alpha^2)^2$, gives a formula previously derived by Talman (1970).

6. Conclusion

The matrix elements between harmonic oscillator eigenfunctions of the operators $\exp(-b^2r^2)$ and $\exp(-s^2p^2/\hbar^2)$ may be evaluated by considering isometric group representations. Since the representation includes the scaling operator, one can also obtain matrix elements between eigenfunctions having different spring constants.

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