Generating two-dimensional oscillator matrix elements sorted by angular momentum

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Abstract
Generating functions are found for two-dimensional harmonic-oscillator integrals. These integrals are classified by angular momentum, permitting inclusion of a constant magnetic field. A generating function is obtained for matrix elements of a Gaussian perturbation, and as an example these are used to compute eigenstates for a particle in a wine bottle-bottom potential. Along with this specific example a straightforward method of generalizing the results is presented.

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1. Introduction

The harmonic-oscillator paradigm in quantum mechanics has a range of applications. Due to their convenient properties, oscillator eigenfunctions often serve as a basis set. For molecular or many-body calculations, the Gaussian basis functions exhibit several advantages over alternatives such as the Slater-type orbitals (Boys 1950). Although the Gaussians do not have the asymptotic forms expected of atomic wavefunctions, either at large or at small radii, the greater efficiency they afford for computing integrals more than compensates for the fact that a large number of Gaussians must be used. In particular, the space of all Gaussian functions of the form

$$\phi(x, a) = A \exp(-x^2/a^2)$$

is closed under products, translations and convolutions. The Fourier transforms are also Gaussians. Matrix elements of functions such as

$$x^n \exp(-x^2/a^2), \qquad x^n e^{-ikx},$$

and so on are related simply enough to the Gaussian integrals so that they can be evaluated easily also (Matthews and Walker 1970). So can the generalizations to two or three dimensions. The oscillator eigenfunctions share these advantages, and have others as well. For example,

eigenfunctions of a given oscillator are naturally orthogonal to one another and can be manipulated easily with the familiar ladder operators a and $a^\dagger$. Even so, explicit calculation of a large number of matrix elements becomes cumbersome, which motivates the use of generating functions.

The hypervirial theorem has been used to obtain recurrence relations for two-centre oscillator matrix elements in one dimension (Morales *et al* 1987, Morales 1987). Soon afterwards Rashid (1989) found generating functions for two-centre oscillator integrals $\langle m|f(a, a^\dagger)|n\rangle$ by transforming the recurrence relations, which he did without the use of the hypervirial theorem. Rashid derived recurrence relations for two-centred matrix elements

$$\int_{-\infty}^{\infty} \psi_m^{(g)*}(x - x_o) f(a, a^\dagger) \psi_n^{(e)}(x) \, dx,$$

in one dimension by purely algebraic methods. This was done for the cases

$$f(a, a^\dagger) = 1, \qquad x^k, \qquad e^{-\rho x}, \qquad e^{-\rho x^2}.$$

In the following, we obtain generating functions for the two-dimensional case using the Weisner method (Weisner 1954, McBride 1971). A complete set of ladder operators is obtained by determining simultaneous eigenvectors of the angular momentum and Hamiltonian operators. Thus, both energy and angular momentum are taken into account by the resulting generating function, which is of a rather simple form. To show the utility of this generating function, we calculate eigenstates of a two-dimensional oscillator with a Gaussian perturbation.

The organization of this paper is as follows. A generating function for two-dimensional oscillator eigenstates, sorted by angular momentum, is constructed in section 2. With this tool the case of an applied constant magnetic field can also be treated. The results of section 2 are used to obtain a generating function for matrix elements of a Gaussian potential in section 3. In addition to the generating function, an explicit formula is given for the general, angle-resolved Gaussian matrix element and specific results are tabulated. The example of a hat potential is treated in section 4. Finally, in the last section, we comment on generalizing to matrix elements of the form $r^{2k} \exp(-r^2/a^2)$.

2. Generating function for two-dimensional oscillator

Consider an isotropic harmonic oscillator with mass m and force constant $m\alpha^2$. The Hamiltonian is

$$H_o = \frac{1}{2m} p^2 + m\alpha^2 r^2. \tag{1}$$

The characteristic length scale is

$$b = \sqrt{\frac{\hbar}{m\alpha}}. \tag{2}$$

When both angular momentum and energy are considered, one finds a complete set of ladder operators as presented in table 1. Each of these operators is chosen so that

$$[L_z, w] = \lambda w \qquad \text{and} \qquad [H, w] = \epsilon w, \tag{3}$$

for particular constants λ and ϵ, so that $v^\dagger$ raises both energy and angular momentum quantum numbers, while $u^\dagger$ raises energy and lowers angular momentum. Four cases are shown. Also, u and v commute. The normalized eigenstate

$$\psi_{n_1,n_2}(x, y) = \frac{(u^\dagger)^{n_1}(v^\dagger)^{n_2}}{\sqrt{n_1! n_2!}} \psi_{0,0}(x, y) \tag{4}$$

Table 1. Complete set of ladder operators.

	λ	ϵ	Operator
1	$+\hbar$	$-\hbar\alpha$	$u = \frac{1}{2}\sqrt{\frac{m\alpha}{\hbar}}\left(x + \mathrm{i}y + \frac{\mathrm{i}}{m\alpha}p_x - \frac{1}{m\alpha}p_y\right)$
2	$-\hbar$	$\hbar\alpha$	$u^{\dagger} = \frac{1}{2}\sqrt{\frac{m\alpha}{\hbar}}\left(x - \mathrm{i}y - \frac{\mathrm{i}}{m\alpha}p_x - \frac{1}{m\alpha}p_y\right)$
3	$-\hbar$	$-\hbar\alpha$	$v = \frac{1}{2}\sqrt{\frac{m\alpha}{\hbar}}\left(x - \mathrm{i}y + \frac{\mathrm{i}}{m\alpha}p_x + \frac{1}{m\alpha}p_y\right)$
4	$+\hbar$	$\hbar\alpha$	$v^{\dagger} = \frac{1}{2}\sqrt{\frac{m\alpha}{\hbar}}\left(x + \mathrm{i}y - \frac{\mathrm{i}}{m\alpha}p_x + \frac{1}{m\alpha}p_y\right)$

has eigenvalues with respect to both L_z and H, namely

$$L_z\psi_{n_1,n_2}(x, y) = \hbar(n_2 - n_1)\psi_{n_1,n_2}(x, y),$$
$$H\psi_{n_1,n_2}(x, y) = (\hbar\alpha(n_1 + n_2 + 1))\psi_{n_1,n_2}(x, y). \tag{5}$$

The ground state $\psi_{0,0}$ annihilated by both u and v is

$$\psi_{0,0}(x, y) = \frac{1}{b\sqrt{\pi}}\exp\left(-\frac{x^2 + y^2}{2b^2}\right). \tag{6}$$

Thus, a convenient generating function would appear to be of the form

$$F(x, y, s, t) = \sum_{n_1,n_2}\frac{1}{\sqrt{n_1!n_2!}}s^{n_1}t^{n_2}\psi_{n_1,n_2}(x, y)$$
$$= \sum_{n_1,n_2}\frac{1}{n_1!n_2!}s^{n_1}t^{n_2}(u^{\dagger})^{n_1}(v^{\dagger})^{n_2}\psi_{0,0}(x, y) = \exp(su^{\dagger} + tv^{\dagger})\psi_{0,0}(x, y). \tag{7}$$

Equation (7) reflects the fact that $[u^{\dagger}, v^{\dagger}] = 0$.

Starting from the $u^{\dagger}$ and $v^{\dagger}$ described in table 1, Weisner's method (Weisner 1955) is employed to obtain a generating function. The strategy is to find canonical variables such that $u^{\dagger}$ and $v^{\dagger}$ are essentially derivatives and then to evaluate equation (7) via the Taylor theorem. We note that the generating function defined in equation (7) is also a coherent state, or a mutual eigenstate of u and v. Characteristics for the two first-order partial differential equations $u\psi_{0,0} = 0$ and $v\psi_{0,0} = 0$ are

$$\xi = \frac{x + \mathrm{i}y}{b\sqrt{2}}, \qquad \xi^* = \frac{x - \mathrm{i}y}{b\sqrt{2}}, \tag{8}$$

or

$$x = \frac{b}{\sqrt{2}}(\xi + \xi^*), \qquad y = \frac{-\mathrm{i}b}{\sqrt{2}}(\xi - \xi^*). \tag{9}$$

In these variables,

$$u^{\dagger} = \frac{1}{\sqrt{2}}\left(\xi^* - \frac{\partial}{\partial\xi}\right) \qquad v^{\dagger} = \frac{1}{\sqrt{2}}\left(\xi - \frac{\partial}{\partial\xi^*}\right). \tag{10}$$

The next step is to relate $u^{\dagger}$ and $v^{\dagger}$ each by gauge transformation to a derivative operator. Thus, suppose one has a function $\mu = \mu(\xi, \xi^*)$ such that

$$u^{\dagger} = -\frac{1}{\sqrt{2}}\frac{1}{\mu}\frac{\partial}{\partial\xi}\mu.$$

Then

$$u^{\dagger} = -\frac{1}{\sqrt{2}}\left(\frac{\partial}{\partial\xi} + \frac{1}{\mu}\frac{\partial\mu}{\partial\xi}\right),$$

comparing this to $u^{\dagger}$ in (10)

$$\frac{1}{\mu}\frac{\partial \mu}{\partial \xi} = -\xi^*,$$

so that the integrating factor μ is

$$\mu = \mathrm{e}^{-\xi\xi^*}.$$

Similarly, one finds the *same* integrating factor for $v^{\dagger}$. Therefore, the ladder operators become

$$u^{\dagger} = \mathrm{e}^{\xi\xi^*}\left(-\frac{1}{\sqrt{2}}\frac{\partial}{\partial \xi}\right)\mathrm{e}^{-\xi\xi^*}, \qquad v^{\dagger} = \mathrm{e}^{\xi\xi^*}\left(-\frac{1}{\sqrt{2}}\frac{\partial}{\partial \xi^*}\right)\mathrm{e}^{-\xi\xi^*}. \tag{11}$$

Equations (11) generalize to

$$(u^{\dagger})^{n_1} = \mathrm{e}^{\xi\xi^*}\left(-\frac{1}{\sqrt{2}}\frac{\partial}{\partial \xi}\right)^{n_1}\mathrm{e}^{-\xi\xi^*}, \qquad (v^{\dagger})^{n_2} = \mathrm{e}^{\xi\xi^*}\left(-\frac{1}{\sqrt{2}}\frac{\partial}{\partial \xi^*}\right)^{n_2}\mathrm{e}^{-\xi\xi^*}. \tag{12}$$

Let $\tilde{F}(\xi, \xi^*, s, t) = F(x(\xi, \xi^*), y(\xi, \xi^*), s, t)$. Inserting the expressions for $(u^{\dagger})^{n_1}$ and $(v^{\dagger})^{n_2}$ one has

$$\tilde{F}(\xi, \xi^*, s, t) = \frac{1}{\mu(\xi, \xi^*)}\exp\left(-\frac{s}{\sqrt{2}}\frac{\partial}{\partial \xi}\right)\exp\left(-\frac{t}{\sqrt{2}}\frac{\partial}{\partial \xi^*}\right)\mu(\xi, \xi^*)\tilde{\psi}_{0,0}(\xi, \xi^*), \tag{13}$$

where

$$\tilde{\psi}_{0,0}(\xi, \xi^*) = \frac{1}{b\sqrt{\pi}}\mathrm{e}^{-\xi\xi^*}. \tag{14}$$

Ultimately, since the exponentiated operators in equation (13) effect a shift in the arguments ξ and ξ^*, this leads to the generating function

$$\tilde{F}(s, t, \xi, \xi^*) = \tilde{\psi}_{0,0}(\xi, \xi^*)\exp\left[2\xi\frac{s}{\sqrt{2}} + 2\xi^*\frac{t}{\sqrt{2}} - st\right],$$

or in the original Cartesian coordinates,

$$F(s, t, x, y) = \psi_{0,0}(x, y)\exp\left[\frac{(x+\mathrm{i}y)s}{b} + \frac{(x-\mathrm{i}y)t}{b}\right]\mathrm{e}^{-st}. \tag{15}$$

Expanding $F(s, t, x, y)$ in powers of s and t and collecting coefficients, one can obtain any desired quantum state.

One may note that the case of an applied magnetic field can be treated without difficulty (Landau and Lifshitz 1981). When we apply a field $\vec{B} = B_o\hat{z}$,

$$H = H_o - \frac{qB_o}{2mc}L_z + \frac{1}{2}m\left(\frac{qB_o}{2mc}\right)^2 r^2. \tag{16}$$

The presence of the field breaks the chiral symmetry of the oscillator and motivates the definitions

$$\omega_b = \frac{qB_o}{2mc}, \tag{17}$$

$$\Omega = \sqrt{\alpha^2 + \omega_b^2}. \tag{18}$$

Thus, the characteristic length is now

$$b = \sqrt{\frac{\hbar}{m\Omega}}. \tag{19}$$

Table 2. Complete set of ladder operators with an applied field.

	λ	ϵ	Operator
1	$+\hbar$	$\hbar(-\Omega - \omega_b)$	$u = \frac{1}{2}\sqrt{\frac{m\Omega}{\hbar}}\left(x + \mathrm{i}y + \frac{\mathrm{i}}{m\Omega}p_x - \frac{1}{m\Omega}p_y\right)$
2	$-\hbar$	$\hbar(+\Omega + \omega_b)$	$u^\dagger = \frac{1}{2}\sqrt{\frac{m\Omega}{\hbar}}\left(x - \mathrm{i}y - \frac{\mathrm{i}}{m\Omega}p_x - \frac{1}{m\Omega}p_y\right)$
3	$-\hbar$	$\hbar(-\Omega + \omega_b)$	$v = \frac{1}{2}\sqrt{\frac{m\Omega}{\hbar}}\left(x - \mathrm{i}y + \frac{\mathrm{i}}{m\Omega}p_x + \frac{1}{m\Omega}p_y\right)$
4	$+\hbar$	$\hbar(+\Omega - \omega_b)$	$v^\dagger = \frac{1}{2}\sqrt{\frac{m\Omega}{\hbar}}\left(x + \mathrm{i}y - \frac{\mathrm{i}}{m\Omega}p_x + \frac{1}{m\Omega}p_y\right)$

The normalized eigenstate $\psi_{n_1,n_2}(x, y)$ is the same as in equation (4), but with parameters deformed to correspond to the transformed ladder operators defined in table 2. Therefore,

$$L_z\psi_{n_1,n_2}(x, y) = \hbar(n_2 - n_1)\psi_{n_1,n_2}(x, y),$$
$$H\psi_{n_1,n_2}(x, y) = (\hbar\omega_b(n_1 - n_2) + \hbar\Omega(n_1 + n_2 + 1))\,\psi_{n_1,n_2}(x, y). \tag{20}$$

Thus, H is deformed continuously from H_o at $\omega_b = 0$ (zero field) and the physical properties deform smoothly as well. The results obtained previously still hold *mutatis mutandis* with α replaced by Ω. Now, however, the energy degeneracy between states with right- and left-handed angular momentum is split by the field as seen in the table.

3. Generating function for matrix elements of a Gaussian potential

A generating function for the matrix elements of $\widehat{V}$ where

$$\langle x, y|\widehat{V}|x, y\rangle = \exp\left(-\frac{x^2 + y^2}{a^2}\right) \tag{21}$$

is

$$G(s, t, p, q) = \langle F(x, y, s, t)|\exp(-r^2/a^2)|F(x, y, p, q)\rangle, \tag{22}$$

where we have used an obvious notational shorthand. One has

$$G(s, t, p, q) = \sum \frac{s^{n_1}t^{n_2}p^{n_3}q^{n_4}}{\sqrt{n_1!n_2!n_3!n_4!}}\langle n_1, n_2|\widehat{V}|n_3, n_4\rangle. \tag{23}$$

By defining the shape parameter

$$\zeta = \frac{a^2}{a^2 + b^2}, \tag{24}$$

and completing the square in the exponent, the integral implied by equation (22) can be evaluated in a simple form:

$$G(s, t, p, q) = \zeta \exp\left[(\zeta - 1)(st + pq) + \zeta(sp + tq)\right]. \tag{25}$$

Equation (25), which gives $G(s, t, p, q)$ in a succinct form, is our principal result. Conservation of angular momentum requires that $n_2 - n_1 = n_4 - n_3$. In view of equation (5), we introduce an angular momentum quantum number $\ell = n_2 - n_1$. Thus, non-vanishing integrals are of the form

$$\langle n_1, n_1 + \ell|\widehat{V}|n_3, n_3 + \ell\rangle. \tag{26}$$

By expanding equation (25),

$$G = \sum_{jkgh} \frac{1}{j!k!g!h!}(\zeta - 1)^{j+k}\zeta^{g+h+1}s^{j+g}t^{j+h}p^{k+g}q^{k+h}, \tag{27}$$

Table 3. Matrix elements $\langle m, m + \ell | \widehat{V} | n, n + \ell \rangle$ for selected ℓ, m and n.

	ℓ	m	n	Gaussian matrix elements
1	0	0	0	ζ
2	0	1	0	$\zeta^2 - \zeta$
3	0	1	1	$2\zeta^3 - 2\zeta^2 + \zeta$
4	0	2	0	$\zeta^3 - 2\zeta^2 + \zeta$
5	0	2	1	$3\zeta^4 - 5\zeta^3 + 3\zeta^2 - \zeta$
6	0	2	2	$6\zeta^5 - 12\zeta^4 + 10\zeta^3 - 4\zeta^2 + \zeta$
7	1	0	0	ζ^2
8	1	1	0	$\sqrt{2}\zeta^3 - \sqrt{2}\zeta^2$
9	1	1	1	$3\zeta^4 - 4\zeta^3 + 2\zeta^2$
10	1	2	0	$\sqrt{3}\zeta^4 - 2\sqrt{3}\zeta^3 + \sqrt{3}\zeta^2$
11	1	2	1	$2\sqrt{6}\zeta^5 - 4\sqrt{6}\zeta^4 + 3\sqrt{6}\zeta^3 - \sqrt{6}\zeta^2$
12	1	2	2	$10\zeta^6 - 24\zeta^5 + 24\zeta^4 - 12\zeta^3 + 3\zeta^2$
13	2	0	0	ζ^3
14	2	1	0	$\sqrt{3}\zeta^4 - \sqrt{3}\zeta^3$
15	2	1	1	$4\zeta^5 - 6\zeta^4 + 3\zeta^3$
16	2	2	0	$\sqrt{6}\zeta^5 - 2\sqrt{6}\zeta^4 + \sqrt{6}\zeta^3$
17	2	2	1	$5\sqrt{2}\zeta^6 - 11\sqrt{2}\zeta^5 + 9\sqrt{2}\zeta^4 - 3\sqrt{2}\zeta^3$
18	2	2	2	$15\zeta^7 - 40\zeta^6 + 44\zeta^5 - 24\zeta^4 + 6\zeta^3$

and comparing to equation (23), one can assign

$$j + g = n_1, \qquad j + h = n_1 + \ell, \qquad k + g = n_3, \qquad k + h = n_3 + \ell.$$

Therefore

$$k = j - n_1 + n_3, \qquad g = n_1 - j, \qquad h = n_1 + \ell - j, \tag{28}$$

and j remains to be summed. Thus, the general matrix element is

$$\langle n_1, n_1 + \ell | \widehat{V} | n_3, n_3 + \ell \rangle$$
$$= \sum_j \frac{\sqrt{(n_1)!(n_1 + \ell)!(n_3)!(n_3 + \ell)!}}{j!(j - n_1 + n_3)!(n_1 - j)!(n_1 + \ell - j)!} (\zeta - 1)^{2j - n_1 + n_3} \zeta^{2n_1 - 2j + \ell + 1}. \tag{29}$$

The range on j is determined by the denominator of equation (29), since where the argument of any one of the factorials goes negative, the denominator becomes infinite and so the coefficient must vanish; thus

$$0 \leqslant j \leqslant \ell + n_1 \qquad \text{and} \qquad n_1 - n_3 \leqslant j \leqslant n_1.$$

Several matrix elements for a Gaussian bump are shown in table 3. Note that ζ contains the effect of an applied field owing to its dependence on b, since when a field is applied, b of equation (2) is replaced as indicated in equation (19).

4. Example of a hat potential

Here, we apply the generating function developed in the previous section to a quadratic potential with Gaussian perturbation. As an example of a rotationally symmetric problem in two dimensions, consider a particle of mass m subject to the potential

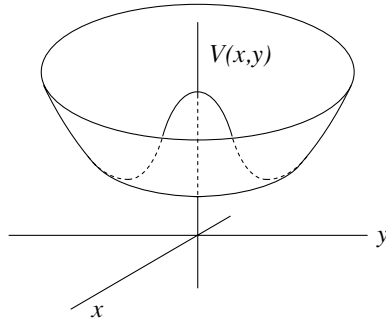$$V(r) = \tfrac{1}{2} m\alpha^2 r^2 + V_o \exp(-r^2/a^2). \tag{30}$$
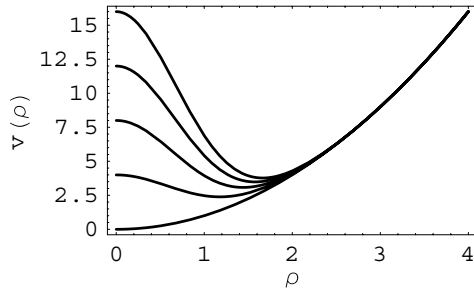
Figure 1. Wine bottle-bottom potential.

Figure 2. Shape for $v_o = 0, 4, 8, 12$ and 16.

With the proper choice of V_o and a, the graph of $V(r)$ versus r resembles a hat or the bottom of a wine bottle. A qualitative sketch of this wine bottle-bottom potential is given in figure 1. Scaling to a dimensionless radial coordinate $\rho = r/a$ yields

$$V(r) = \tfrac{1}{2}m\alpha^2 a^2(\rho^2 + v_o \exp(-\rho^2)), \tag{31}$$

With

$$v_o = \frac{2V_o}{m\alpha^2 a^2},$$

so that v_o is a dimensionless version of the potential strength V_o. The shape of the resulting dimensionless form

$$v(\rho) = \rho^2 + v_o \exp(-\rho^2)$$

is shown in figure 2 for several values of v_o. When $v_o > 1$, the minimum moves away from 0 to $\rho = \sqrt{\ln(v_o)}$. The Hamiltonian H is such that

$$\langle m + \ell, m|H|n + \ell, n \rangle = \hbar\alpha(2n + \ell + 1)\delta_{mn} + \hbar\alpha v \langle m + \ell, m| \exp(-r^2/a^2)|n + \ell, n \rangle, \tag{32}$$

with $v = a^2 v_o/b^2$. Figure 3 shows the energy levels as a function of v for the case $\zeta = 3/4$ with ζ as defined in equation (24). Energies E are in units of $\hbar\alpha$.

The energies shown in figure 3 are found from nine separate variational calculations, one for each angular quantum number from $\ell = 0$ to $\ell = 8$ and each done in a basis of 16 ℓ-projected oscillator functions. The energies for $\pm\ell$ are degenerate. For small v the levels split linearly, with residual $\pm\ell$ degeneracy, while for large v one can expand in a harmonic
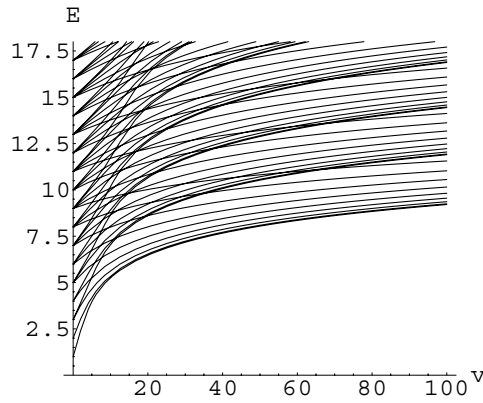
Figure 3. Energy levels of the wine bottle-bottom in units of $\hbar\alpha$ as a function of central height in the same units.

approximation about the effective minimum potential. So for $0 < \zeta < 1$ and $v \gg 1$,

$$E \approx \hbar\alpha\sqrt{2\ln(v)}\left(n + \frac{1}{2}\right) + \frac{1}{2}\frac{\zeta}{1-\zeta}\hbar\alpha(1 + \ln(v)) + \hbar\alpha\frac{1-\zeta}{\zeta}\frac{\ell^2}{\ln(v)}. \tag{33}$$

Applying a magnetic field is straightforward. In view of the above discussion,

$$\langle m + \ell, m|H|n + \ell, n\rangle = \hbar\Omega(2n + \ell + 1)\delta_{mn} + v\hbar\alpha\langle m + \ell, m|\exp(-r^2/a^2)|n + \ell, n\rangle. \tag{34}$$

So the matrix elements are deformed by an amount depending on ℓ, and in a rather simple way on ω_o, i.e. on the field applied. The magnetic field lifts the $\pm\ell$ degeneracy.

5. Generating function for matrix elements of $r^{2k}\exp(-r^2/a^2)$

With the generating function developed as in the previous sections, it is straightforward to calculate a number of related results. Here we give just one illustration. For integrals of the form

$$\langle m, m + \ell|r^{2k}\,e^{-r^2/a^2}|n, n + \ell\rangle \tag{35}$$

it suffices to evaluate the generating function

$$\begin{aligned}
K(s, t, p, q, \sigma) &= \sum \frac{(-\sigma)^k}{k!}\frac{s^{n_1}t^{n_2}p^{n_3}q^{n_4}}{\sqrt{n_1!n_2!n_3!n_4!}}\langle n_1, n_2|r^{2k}\widehat{V}|n_3, n_4\rangle \\
&= \sum \frac{s^{n_1}t^{n_2}p^{n_3}q^{n_4}}{\sqrt{n_1!n_2!n_3!n_4!}}\langle n_1, n_2|\exp(-\sigma r^2 - r^2/a^2)|n_3, n_4\rangle.
\end{aligned} \tag{36}$$

One sees that this expression can be found from the function $G(s, t, p, q)$ defined in equation (23) by replacing $1/a^2$ in the exponent with $1/a^2 + \sigma$. But this is the same thing as replacing ζ in the result shown in equation (25) by

$$\zeta(\sigma) = \frac{\zeta}{1 + \zeta\sigma b^2} \tag{37}$$

which gives

$$K(s, t, p, q, \sigma) = \frac{\zeta}{\zeta\sigma b^2 + 1}\exp\left(-(pq + st) + \frac{(st + pq + sp + tq)\zeta}{\zeta\sigma b^2 + 1}\right). \tag{38}$$

6. Summary

By constructing simultaneous ladder operators of energy and angular momentum, as shown in table 1, it is not difficult to derive the generating function $F(x, y, s, t)$ for the simultaneous eigenfunctions of H and L_z given in equation (15). Upon integrating the product of two copies of this generating function with the symmetrical Gaussian $\exp(-r^2/a^2)$, we have another generating function $G(s, t, p, q)$ in equation (25) for the Gaussian matrix elements. A concise formula for matrix elements is given in equation (29). To illustrate the utility of these, we have computed energy levels of a wine bottle-bottom potential as a function of a shape parameter ζ as described in section 3. The simple form of $G(s, t, p, q)$ in equation (25) makes it quite useful in calculations with an oscillator basis in problems with cylindrical symmetry. Related generating functions such as $K(s, t, p, q, \sigma)$ in section 5 follow easily from the formula for $G(s, t, p, q)$ and are also useful. We have found it convenient to have simple Mathematica functions for obtaining the desired matrix elements directly by evaluating Taylor series coefficients.

References

Boys S F 1950 *Proc. R. Soc.* **200** 542–54
Landau L and Lifshitz E 1981 *Quantum Mechanics* (Oxford: Pergamon) p 454
Matthews J and Walker R 1970 *Mathematical Methods of Physics* (Boston, MA: Addison-Wesley) p 58
McBride E 1971 *Obtaining Generating Functions* ed B Coleman (New York: Springer) p 25
Morales J 1987 *Phys. Rev.* A **36** 4101–3
Morales J, Lopez-Bonilla J and Palma A 1987 *J. Math. Phys.* **28** 1032–5
Rashid M 1989 *J. Math. Phys.* **30** 398
Weisner L 1955 *Pac. J. Math.* **5** 1033–9