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Moments of the radial density distribution

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Abstract. The matrix elements of powers of r^2 are evaluated in the basis of radial wavefunctions of a three-dimensional harmonic oscillator as a terminating type of generalised hypergeometric function ${}_3F_2$. They are employed to calculate the low-order moments of the radial density distribution. The form of radial density distribution for large values of oscillator quanta are given.

The matrix elements of the radial operator are commonly used in many areas of physics. For the harmonic oscillator potential they are integrals of two Laguerre polynmials with some powers of the radial distance and Gaussian weight function. In earlier studies Gargaro and Onley (1970) investigated such integrals in connection with the matrix element of a relativistic electron in a Coulomb field. They were expressed in terms of generalised hypergeometric functions ${}_3F_2$ which are terminating types in the order of Laguerre polynomials. These expressions are not suitable when one wants to study the moments of the radial distribution where one has to sum over orbital angular momenta and the radial quantum number. Our aim here is to derive a new expression for the radial matrix elements which is of a terminating type in the power of the radial distance.

Let us consider the eigenvalue equation for the three-dimensional harmonic oscillator which is given by

$$(-\tfrac{1}{2}\nabla^2+\tfrac{1}{2}r^2)\psi(r,\theta,\phi)=E\psi(r,\theta,\phi) \tag{1}$$

where we have employed the units in which $\hbar^2/m=k=1$. The eigenfunctions ψ are given by (Morse and Feshbach 1953)

$$\psi=R_{nl}(r)\,Y_{lm}(\theta,\phi) \tag{2}$$

and the energy eigenvalues E are given by

$$E_n=(N+\tfrac{3}{2}) \tag{3}$$

where N denotes the oscillator quanta and can take on values $N=0,1,2,\ldots$, l denotes orbital angular momentum and has values $0, 1, 2, \ldots$ and m is its projection. The quantum number n which is related to the number of nodes in the radial wavefunction can take on values $n=1, 2, \ldots$. For a given N, quantum numbers n, l can take all possible values given by the relation

$$N=2(n-1)+l. \tag{4}$$

We are here using nuclear spectroscopy (Preston 1962) convention for the quantum number n.

The radial wavefunctions $R_{nl}(r)$ are given by (Morse and Feshbach 1953)

$$R_{nl}(r) = N_{nl} \exp(-\tfrac{1}{2}r^2) r^l L_{n-1}^{(l+1/2)}(r^2) \tag{5}$$

where $L_{n-1}^{(l+1/2)}$ is the generalised Laguerre polynomial and N_{nl} is determined by the normalisation condition

$$\int_0^\infty R_{nl}^2(r) r^2 \, \mathrm{d}r = 1. \tag{6}$$

Using the substitution $r^2 = x$, the matrix elements of the powers of r^2 in the basis of R_{nl} can be obtained by evaluating the integral I given by

$$I = \int_0^\infty \exp(-x) x^\mu L_{k_1}^{(\nu_1-1)}(x) L_{k_2}^{(\nu_2-1)}(x) \, \mathrm{d}x. \tag{7}$$

We shall use the generating function (Abramowitz and Stegun 1965) for the generalised Laguerre polynomials to evaluate this integral. Thus I can be written as

$$I = \frac{1}{(2\pi \mathrm{i})^2} \oint \oint \mathrm{d}z \, \mathrm{d}\xi \int_0^\infty \mathrm{d}x \exp\left[-\left(1 - \frac{z}{z-1} - \frac{\xi}{\xi-1}\right)\right] x^\mu$$
$$\times z^{-k_1-1}(1-z)^{-\nu_1} \xi^{-k_2-1}(1-\xi)^{-\nu_2}.$$

Carrying out the integral over x and after some simplification we can write I as

$$I = \Gamma(\mu+1) \frac{1}{(2\pi \mathrm{i})^2} \oint \oint \mathrm{d}z \, \mathrm{d}\xi (1-z)^{-\nu_1+\mu+1} (1-\xi)^{-\nu_2+\mu+1} (1-z\xi)^{-\mu-1}.$$

Expanding $(1-z\xi)^{-\mu-1}$, putting in the value of $L_k^{(\alpha)}(0)$ and after a minor simplification we finally arrive at the following expression for I:

$$I = \frac{\Gamma(\mu+k_1+1)\Gamma(k_2-k_1+\nu_2-\mu-1)}{\Gamma(k_1+1)\Gamma(k_2-k_1+1)\Gamma(\nu_2-\mu-1)}$$
$$\times {}_3F_2(-k_1, \nu_1-\mu-1, k_2-k_1+\nu_2-\mu-1; -k_1-\mu, k_2-k_1+1; 1) \tag{8}$$

where ${}_3F_2$ is the generalised hypergeometric function (Bateman 1953). In writing expression (8) we have taken $k_1 \leqslant k_2$.

We shall next apply expression (8) to find the low-order moments of the radial density distribution.

Consider a closed-shell nucleus and assume that the nucleons fully occupy oscillator levels up to $N = N_0$. The density of nucleons $\rho(\bar{r})$ can then be written as

$$\rho(\bar{r}) = \sum_{i=1}^{A} \phi_i^2(\bar{r}) \tag{9}$$

where ϕ_i are single-nucleon wavefunctions. They are given by a product of ψ_i of equation (2) and the spin-isospin wavefunction. $\rho(\bar{r})$ is normalised so that

$$\int \rho(\bar{r}) \, \mathrm{d}\bar{r} = A \tag{10}$$

where A is the total number of nucleons. Since we are considering closed-shell nuclei, $\rho(\bar{r})$ is a function of r only. Integrating over angular variables and carrying through summation over spin and isospin we can write

$$4\pi\rho(r) = 4 \sum_{N,n,l} R_{nl}^2(r)(2l+1) \tag{11}$$

where the sum is carried out over the quantum numbers n, l, subject to the constraint given by (4) and over N from 0 to N_0. The moments of (r^2) are defined by

$$\langle r^{2q}\rangle = \int_0^\infty \rho(r) r^{2q+2}\,\mathrm{d}r\left(\int_0^\infty \rho(r) r^2\,\mathrm{d}r\right)^{-1} \qquad q=1,2,\ldots. \tag{12}$$

Since $\rho(r)$ is a sum of R_{nl}^2, we need integrals of R_{nl}^2 with powers of r^2, so that the sums in expression (11) can be carried out.

Let us consider one such integral given by

$$J = \int_0^\infty R_{nl}^2 r^6\,\mathrm{d}r \tag{13}$$

which will be needed for the second moment $\langle r^4\rangle$. Using expressions (5), (6), (8) we find that it is given by

$$J = \frac{\Gamma(n+l+\frac{5}{2})}{\Gamma(n+l+\frac{1}{2})}\,{}_3F_2(-n+1,-2,-2;-n-l-\tfrac{3}{2},1;1). \tag{14}$$

Since ${}_3F_2$ has one of its parameters as -2, it terminates only after three terms to give

$$J = 6n^2+6nl-3n+l^2-2l+\tfrac{3}{4}. \tag{15}$$

One can now easily carry out summations over l, n.

Thus we find that the first and second moment of r^2 for closed-shell nuclei in which A nucleons are fully occupying oscillator energy levels up to $N=N_0$ are given by

$$\langle r^2\rangle = \tfrac{3}{4}(N_0+2) \tag{16a}$$

$$\langle r^4\rangle = \tfrac{3}{4}(N_0^2+4N_0+5). \tag{16b}$$

It is easy to see from expression (16) that

$$\frac{\langle r^4\rangle}{\langle r^2\rangle^2} = \frac{4}{3}\left(1+\frac{1}{(N_0+2)^2}\right) \tag{17}$$

which becomes $\frac{4}{3}$ if $N_0 \gg 1$.

The radial distribution $\rho(r)$ which gives this ratio for large N_0 is found to be

$$\rho(r) = \frac{2}{3\pi^2}[2(N_0+2)-r^2]^{3/2}. \tag{18}$$

We would now like to make a few remarks. The first is that even though quite a few expressions exist in the literature for the integrals given by expression (7), they are all of terminating type in the index k_1, k_2 of the Laguerre polynomial. What we have given here for the first time is an expression which is of terminating type in the power of r. As shown above, such expressions enable us to carry out further summations over the quantum numbers n, l. Secondly, since there are a large number of transformations which connect various ${}_3F_2$ one could have tried to find such an expression starting from one of the known expressions. Because of the large number of transformations such a search would be quite a task to perform. Our last remark is that there are more recent interests in the problem of radial moments as given by Roy *et al* (1988) which enhance the importance of the present study of the radial matrix elements.

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