Working in the Spherical Harmonic Oscillator Basis

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The purpose of these notes is to help you computing the matrix elements of the Minnesota potential in the harmonic oscillator basis.

1 The Spherical Harmonic Oscillator Basis

In this section, we look at the eigenstates of the spherical quantum harmonic oscillator

$$\hat{H}_0 = \frac{\boldsymbol{p}^2}{2m} + \frac{1}{2}m\omega\boldsymbol{r}^2 \tag{1}$$

in the special case of spherical symmetry.

1.1 Eigenstates of the Harmonic Oscillator

General Form - The solutions to the Schrödinger equation for an arbitrary central potential in spherical symmetry are entirely characterized by the quantum numbers n, ℓ, j and m; the wave-functions factorize according to

$$\boxed{\psi_{n\ell jm}(r,\theta,\varphi) = R_{n\ell}(r)\mathfrak{Y}_{\ell jm}(\theta,\varphi)} \tag{2}$$

where $R_{n\ell}(r)$ is the radial wave-function and $\mathfrak{Y}_{\ell jm}(\theta,\varphi)$ are the solid harmonics. The solid harmonics ℓ, j, m correspond to the tensor product of the spherical harmonics $Y_{\ell m_\ell}(\theta,\varphi)$ with the spin functions χ_{sm_s},

$$\mathfrak{Y}_{\ell jm}(\theta,\varphi) = \left[Y_{\ell m_\ell}(\theta,\varphi) \otimes \chi_{sm_s}\right]_{jm}. \tag{3}$$

More explicitely, this can be re-written

$$\mathfrak{Y}_{\ell jm}(\theta,\varphi) = \sum_{m_s=\pm 1/2} C^{jm}_{\ell m_\ell, sm_s} Y_{\ell m_\ell}(\theta,\varphi), \chi_{sm_s} \tag{4}$$

where the symbols $C^{jm}_{\ell m_\ell, sm_s}$ are the Clebsch-Gordan coefficients.

Radial Function for the Harmonic Oscillator - In the case where the potential is the harmonic oscillator, the radial wave function $R_{n\ell}(r)$ becomes

$$\boxed{R_{n\ell}(r) = A_{n\ell} e^{-\xi^2/2} \xi^\ell L_n^{\ell+1/2}(\xi^2)} \tag{5}$$

where $\xi = br$ is a dimensionless variable and $b = \sqrt{m\omega/\hbar}$ is the oscillator length. The quantities $L_n^{\ell+1/2}$ are the generalized Laguerre polynomials. In Eq. (5), $A_{n\ell}$ is a normalization constant. To determine it, we use the orthonormality of the wave functions $\psi_{n\ell jm}$ and find

$$\boxed{A_{n\ell} = \sqrt{2b^3} \sqrt{\frac{n!}{\Gamma(n+\ell+3/2)}}} \tag{6}$$

1.2 Generalized Laguerre Polynomials

Recurrence Relation - The generalized Laguerre polynomials verify the following recurrence relations (Abramowitz, 22.7.29, 22.7.30)

$$L_n^{(\alpha+1)}(x) = \frac{1}{x}\left[(x-n)L_n^{(\alpha)}(x) + (\alpha+n)L_{n-1}^{(\alpha)}(x)\right] \tag{7}$$

$$L_n^{(\alpha-1)}(x) = L_n^{(\alpha)}(x) - L_{n-1}^{(\alpha)}(x), \tag{8}$$

where n is an integer, $n \in \mathbb{N}$, and α is a real number. In the following, we will only need α half-integer. The two relations (7)-(8) are equivalent to

$$L_n^{(\alpha+1)}(x) = \frac{1}{x}\left[(x+\alpha)L_n^{(\alpha)}(x) - (\alpha+n)L_n^{(\alpha-1)}(x)\right]. \tag{9}$$

The first two polynoms are obtained from

$$L_n^{(-1/2)}(x) = \frac{(-1)^n}{n!2^n} H_{2n}(\sqrt{x}) \tag{10}$$

$$L_n^{(+1/2)}(x) = \frac{(-1)^n}{n!2^{n+1}} H_{2n+1}(\sqrt{x}) \tag{11}$$

where $H_n(x)$ is the Hermite polynomials of order n.

Orthonormality - The generalized Laguerre polynomials verify the following orthonormality condition

$$\boxed{\int_0^{+\infty} e^{-u} u^\alpha L_n^{(\alpha)}(u) L_{n'}^{(\alpha)}(u) du = \delta_{nn'} \frac{\Gamma(n+\alpha+1)}{n!}}, \tag{12}$$

for $\alpha > -1$ and $n \in \mathbb{N}$. The Gamma function is, for any integer k (Abramowitz, 6.1.12),

$$\Gamma\left(k+\frac{1}{2}\right) = \frac{1 \times 3 \times \cdots \times (2k-1)}{2^k} \Gamma\left(\frac{1}{2}\right) \tag{13}$$

which can be recast into

$$\Gamma\left(k+\frac{1}{2}\right) = \frac{(2k)!}{2^{2k}p!} \Gamma\left(\frac{1}{2}\right) \tag{14}$$

with $\Gamma(1/2) = \sqrt{\pi}$.

2 Matrix Elements of the Hamiltonian

We now move to the problem of computing the matrix elements of the Minnesota Hamiltonian in the HO basis. Recall that the Hamiltonian reads

$$\hat{H} = \sum_{ab} t_{ab} c_a^\dagger c_b + \frac{1}{2} \sum_{abcd} \bar{v}_{abcd} c_a^\dagger c_b^\dagger c_d c_c, \tag{15}$$

with

$$\bar{v}_{abcd} = \int d^3\boldsymbol{r}_1 \int d^3\boldsymbol{r}_2 \; \phi_a^*(x_1)\phi_b^*(x_2)\hat{V}\left(1 - \hat{P}_\sigma \hat{P}_r\right)\phi_c^*(x_1)\phi_d(x_2) \tag{16}$$

with a a generic notation for $a \equiv (n_a, \ell_a, j_a, m_a)$.

2.1 Matrix of the Kinetic Energy Operator

We give below, without demonstration, the matrix elements of the kinetic energy operator, i.e., the elements t_{ac}. By virtue of the spherical symmetry, we have

$$t_{ac} = \langle a|\hat{T}|c\rangle = \langle n_a\ell_a j_a m_a|\hat{T}|n_c\ell_c j_c m_c\rangle = \delta_{\ell_a\ell_c}\delta_{j_a j_c}\delta_{m_a m_c}\langle n_a\ell_a j_a m_a|\hat{T}|n_c\ell_a j_a m_a\rangle \tag{17}$$

In practice, straightforward but somewhat lengthy calculations (involving various tricks from angular momentum algebra) give

$$\boxed{\begin{array}{ll}
\langle n_a\ell_a j_a m_a|\hat{T}|n_c\ell_a j_a m_a\rangle = \frac{1}{2}\hbar\omega\left(N + \frac{3}{2}\right) & \text{for } n_a = n_c \\
\langle n_a\ell_a j_a m_a|\hat{T}|n_c\ell_a j_a m_a\rangle = \frac{1}{2}\hbar\omega\sqrt{n_c(n_c+\ell_a)} & \text{for } n_a = n_c - 1 \\
\langle n_a\ell_a j_a m_a|\hat{T}|n_c\ell_a j_a m_a\rangle = \frac{1}{2}\hbar\omega\sqrt{n_a(n_a+\ell_a)} & \text{for } n_a = n_c + 1
\end{array}}$$

2.2 Gauss-Laguerre Quadratures

Presentation - Gauss quadratures are general mathematical methods used to compute integrals of a function. They are based on the properties of orthogonal polynomials and come in several variants. The Gauss-Laguerre quadrature formula reads

$$\int_0^{+\infty} x^\alpha e^{-x} f(x)dx = \sum_{n=1}^{N_q} w_n f(x_n) + R_{N_q}, \tag{18}$$

where the weights w_n are given by

$$w_n = \frac{\Gamma(n+\alpha+1)x_n}{n!(n+1)^2\left[L_{n+1}^\alpha(x_n)\right]^2}, \tag{19}$$

the nodes x_n are the zeros of the generalized Laguerre polynomials, and R_{N_q} is a remainder. The integer N_q is the order of the quadrature.

The essential property of all types of Gauss quadrature is that the quadrature formula is exact *if $f(x)$ is a polynomial of order $p \leq 2N_q - 1$, that is:*

$$\int_0^{+\infty} x^\alpha e^{-x} f(x) dx = \sum_{n=1}^{N_q} w_n f(x_n).$$

Example - To illustrate how useful quadrature formula can be in practice, consider the calculation of the radial integral giving the matrix element of some operator $\hat{O}(r)$ in spherical symmetry. For the sake of simplicity, let us assume that $\hat{O}(r)$ does not contain differential operators for the time being. We have to compute something like

$$\langle n_a|\hat{O}(r)|n_c\rangle \propto \int_0^{+\infty} r^2 dr \times e^{-\xi^2/2}\xi^{\ell_a} L_{n_a}^{\ell_a+1/2}(\xi^2) \times \hat{O}(r) \times e^{-\xi^2/2}\xi^{\ell_a} L_{n_c}^{\ell_a+1/2}(\xi^2), \tag{20}$$

which can be simplified into something like

$$\langle n_a|\hat{O}(r)|n_c\rangle \propto \int_0^{+\infty} u^\alpha e^{-u} \hat{O}(u) L_{n_a}^\alpha(u) L_{n_c}^\alpha(u) du, \quad \alpha = \ell_a + 1/2 \tag{21}$$

Depending on the properties of the operator $\hat{O}(r)$, we can try to choose the order of the quadrature N_q such that these integrations are exact.

2.3 Numerical Implementations

Fortran - We can provide you with ready-to use routines returning the nodes and weights of Gauss-Laguerre quadratures.

C/C++ -

Python - The `scipy` package provides an entire module on Laguerre polynomials, including a class. Most importantly, it provides the function `laggaus` which return the nodes and weights of Gauss-Laguerre quadrature

Mathematica -