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

\[ \hat{H}_0 = \frac{p^2}{2m} + \frac{1}{2}m\omega r^2 \]  

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 \( n, \ell, j \) and \( m \); the wave-functions factorize according to

\[ \psi_{n\ell jm}(r,\theta,\varphi) = R_{\ell m}(r)Y_{\ell jm}(\theta,\varphi) \]  

where \( R_{\ell m}(r) \) is the radial wave-function and \( Y_{\ell jm}(\theta,\varphi) \) are the solid harmonics. The solid harmonics \( \ell, j, m \) correspond to the tensor product of the spherical harmonics \( Y_{\ell m}(\theta,\varphi) \) with the spin functions \( \chi_{s_m} \),

\[ Y_{\ell jm}(\theta,\varphi) = [Y_{\ell m}(\theta,\varphi) \otimes \chi_{s_m}]_{jm}. \]

More explicitely, this can be re-written

\[ Y_{\ell jm}(\theta,\varphi) = \sum_{m_s=\pm 1/2}^{} C_{\ell m_s m_s}^{jm} Y_{\ell m}(\theta,\varphi), \chi_{s_m} \]  

where the symbols \( C_{\ell m_s m_s}^{jm} \) 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

$$R_{n\ell}(r) = \frac{A_{n\ell}}{b^{3/2}} \xi^{\ell} e^{-\xi^2/2} L_n^{\ell+1/2}(\xi^2)$$

where $\xi = r/b$ is a dimensionless variable and $b = \sqrt{\hbar/(m\omega)}$ is the oscillator length (in fm). 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

$$A_{n\ell} = \frac{2^{n+\ell+2} n!}{\pi^{1/2} (2n + 2\ell + 1)!!}$$

1.2 Generalized Laguerre Polynomials

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

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

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

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

$$L_n^{(\alpha+1)}(x) = \frac{1}{x} [(x + \alpha) L_n^{(\alpha)}(x) - (\alpha + n) L_{n-1}^{(\alpha)}(x)].$$

The first two polynomials are obtained from

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

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

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

Orthonormality - The generalized Laguerre polynomials verify the following orthonormality condition

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

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

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

(13)
which can be recast into
\[ \Gamma \left( k + \frac{1}{2} \right) = \frac{(2k)!}{2^{2k}p!} \Gamma \left( \frac{1}{2} \right) \] (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
\[ \hat{H} = \sum_{ab} t_{ab} c_a^\dagger c_b + \frac{1}{2} \sum_{abcd} \bar{v}_{abcd} c_a^\dagger c_b c_c c_d, \] (15)
with the antisymmetrized matrix elements defined by
\[ \bar{v}_{abcd} = \int d^3r_1 \int d^3r_2 \phi_a^*(x_1)\phi_b^*(x_2) \hat{V} \left( 1 - \hat{P}_x \hat{P}_r \right) \phi_c^*(x_1)\phi_d(x_2) \] (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
\[ t_{ac} = \langle a | \hat{T} | c \rangle = \langle n_a \ell_a j_a | n_c \ell_c j_c m_c \rangle = \delta_{\ell_a \ell_c} \delta_{j_a j_c} \delta_{m_a m_c} \langle n_a \ell_a j_a m_a | \hat{T} | n_c \ell_a j_a m_a \rangle \] (17)
In practice, straightforward but somewhat lengthy calculations (involving various tricks from angular momentum algebra) give

<table>
<thead>
<tr>
<th>Case</th>
<th>Expression</th>
</tr>
</thead>
<tbody>
<tr>
<td>( n_a = n_c )</td>
<td>( \frac{1}{2} \hbar \omega \left( N + \frac{3}{2} \right) )</td>
</tr>
<tr>
<td>( n_a = n_c - 1 )</td>
<td>( \frac{1}{2} \hbar \omega \sqrt{n_c(n_c + \ell_a + 1/2)} )</td>
</tr>
<tr>
<td>( n_a = n_c + 1 )</td>
<td>( \frac{1}{2} \hbar \omega \sqrt{n_a(n_a + \ell_a + 1/2)} )</td>
</tr>
</tbody>
</table>

In this expression, \( N = 2n + \ell \) is the main oscillator number.

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

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

(18)

where the weights $w_n$ are given by

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

(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

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

(20)

which can be simplified into something like

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

(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.