Lanczos Bound-state Calculation Code

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(Dated: June 11, 2013)

I. INTRODUCTION

This document contains both documentation concerning the Lanczos Bound-state Calculation Code as well as information about the underlying theory.

II. THEORY

It should be noted that it is possible that one could define a combined basis $|\gamma\rangle$ that represents $|\gamma\rangle = |\alpha\beta\rangle = |\alpha\rangle\,|\beta\rangle$ such that $\gamma[\alpha,\beta]$ in a similar manner to that done with $n[l,m]$ for the $|n\rangle = |lm\rangle$ Tesseral Harmonic basis.

We also may want to test out a specialized code (either in terms of type of rotor or the spin isomers) versus a generalized code (use the symmetrizing operator to select out the even and odd states?) and see which is computationally more efficient.

The Colbert-Miller Formulae will be used for the translational basis and the Wigner functions could possibly be used for the Asymmetric Top ($e^{im\phi}d^J_{MK}(\theta)e^{ik\chi}$).

A. Hamiltonian

It should be noted that one may be able to define a symmetrizing operator that will allow one to select out the ortho, para or spinless states from the Hamiltonian when calculating the Krylov Subspace. The operator would act as follows

$$\begin{aligned} w &= \hat{S}\hat{H}v \\ w_{para} &= \hat{S}_{even}\hat{H}v \\ w_{ortho} &= \hat{S}_{odd}\hat{H}v \\ w_{spinless} &= \hat{S}_{all}\hat{H}v \end{aligned}$$

B. Basis States

1. Rotor Bases

a. Linear Rotor For the linear rotor, the tesseral spherical harmonics will be used as the basis states and are defined as follows (taken from `http://en.wikipedia.org/wiki/Spherical_harmonics`):

$$Y_{lm}(\theta,\phi) = \begin{cases} \frac{1}{\sqrt{2}}\left(Y_l^m(\theta,\phi) + (-1)^m Y_l^{-m}(\theta,\phi)\right) & \text{if } m>0 \\ Y_l^0(\theta,\phi) & \text{if } m=0 \\ \frac{1}{i\sqrt{2}}\left(Y_l^{-m}(\theta,\phi) - (-1)^m Y_l^m(\theta,\phi)\right) & \text{if } m<0 \end{cases} \tag{1}$$

$$= \begin{cases} \sqrt{2}N_{(l,m)}P_l^m(\cos\theta)\cos m\phi & \text{if } m>0 \\ Y_l^0(\theta,\phi) & \text{if } m=0 \\ \sqrt{2}N_{(l,|m|)}P_l^{|m|}(\cos\theta)\sin|m|\phi & \text{if } m<0 \end{cases} \tag{2}$$

where $N_{(l,m)}$ is a normalization constant and is

$$N_{(l,m)} \equiv \sqrt{\frac{1}{2\pi}}\sqrt{\frac{(2l+1)}{2}\frac{(l-m)!}{(l+m)!}} \tag{3}$$

Note that we incorporate the Condon-Shortley phase in $N_{(l,m)}$, so that

$$N_{(l,m)} \equiv (-1)^m\sqrt{\frac{1}{2\pi}}\sqrt{\frac{(2l+1)}{2}\frac{(l-m)!}{(l+m)!}} \tag{4}$$

$Y_l^m(\theta,\phi)$ are the Laplace Spherical Harmonics and are

$$Y_l^m(\theta,\phi) = N_{(l,m)} P_l^m(\cos\theta)\, e^{im\phi} \tag{5}$$

P_l^m are the associated Legendre polynomials of non-negative m, defined as

$$P_l^m(x) = (-1)^m \left(1-x^2\right)^{\frac{m}{2}} \frac{d^m}{dx^m}\left(P_l(x)\right) \tag{6}$$

where $P_l(x)$ are the Legendre Polynomials, expressed using Rodrigues' formula:

$$P_l(x) = \frac{1}{2^l l!}\frac{d^l}{dx^l}[\left(x^2-1\right)^l] \tag{7}$$

In practise, the associated Legendre Polynomials ($P_l^m(x)$) are calculated by first calculating

$$P_l^l(x) = (2l-1)\, P_{l-1}^{l-1}(x)\sqrt{1-x^2}$$

for $l=1$ to $l=l_{max}$, where $P_0^0=1$.

Then, the associated Legendre Polynomials are calculated for $m=0$ to $m=l_{max}-1$ and for $l=1$ to $l=l_{max}$ as follows

$$P_m^{l+1}(x) = \frac{[(2l+1)\, x P_m^l(x) - (l+m)\, P_m^{l-1}(x)]}{l-m+1} \tag{8}$$

where $P_m^{l-1}(x)=0$ if $l-1<m$.

1. Legendre Polynomial Recursion Relations From Abramowitz and Stegun, pg.334, the Legendre Polynomials can be generated using the following recurrence relations, where

$$\begin{array}{l}
\{\nu|\nu\epsilon\mathbb{C}\} \\
\{\mu|\mu\epsilon\mathbb{C}\} \\
\{n|n\geq 0, n\epsilon\mathbb{Z}\} \\
\{m|m\geq 0, m\epsilon\mathbb{Z}\} \\
\{z|z\epsilon\mathbb{C}\} \\
\{x|x\epsilon\mathbb{R}\}
\end{array}$$

If the degree (ν) is varying,

8.5.3:

$$(\nu-\mu+1)\, P_{\nu+1}^{\mu}(z) = (2\nu+1) z P_\nu^\mu(z) - (\nu+\mu) P_{\nu-1}^{\mu}(z) \tag{9}$$

8.5.4:

$$(z^2-1)\frac{dP_\nu^\mu(z)}{dz} = \nu z P_\nu^\mu - (\nu+\mu) P_{\nu-1}^{\mu}(z) \tag{10}$$

If the order (μ) is varying,

8.5.1:

$$P_\nu^{\mu+1}(z) = \sqrt{z^2-1}[(\nu-\mu) z P_\nu^\mu(z) - (\nu+\mu) P_{\nu-1}^{\mu}(z)] \tag{11}$$

8.5.2:

$$(z^2-1)\frac{dP_\nu^\mu(z)}{dz} = (\nu+\mu)(\nu-\mu+1)\sqrt{z^2-1} P_\nu^{\mu-1}(z) - \mu z P_\nu^\mu(z) \tag{12}$$

If the order (μ) and the degree (ν) are varying,

8.5.5:

$$P_{\nu+1}^{\mu}(z) = P_{\nu-1}^{\mu}(z) + (2\nu+1)\sqrt{z^2-1} P_\nu^{\mu-1}(z) \tag{13}$$

It should also be noted that (A&S pg.333 8.4.1 and 8.4.3)

$$P_0^0(z) = 1 \tag{14}$$
$$P_1^0(z) = z \tag{15}$$

and (A&S pg.333 8.2.1)

$$P_{-\nu-1}^{\mu}(z) = P_{\nu}^{\mu}(z) \tag{16}$$

For the system used here, μ can be set to m, ν to n, and z to x, resulting in:
If the degree (n) is varying,

$$(n-m+1)\,P_{n+1}^m\,(x) = (2n+1)xP_n^m(x) - (n+m)P_{n-1}^m(x) \tag{17}$$

$$(x^2-1)\frac{dP_n^m(x)}{dx} = nxP_n^m - (n+m)P_{n-1}^m(x) \tag{18}$$

and Bonnet's Recursion Formula if $m = 0$ (from `http://en.wikipedia.org/wiki/Legendre_polynomials`)

$$(n+1)\,P_{n+1}\,(x) = (2n+1)xP_n(x) - nP_{n-1}(x) \tag{19}$$

from this, the corresponding formula for the derivative is found to be (from `http://en.wikipedia.org/wiki/Legendre_polynomials`)

$$(x^2-1)\frac{dP_n(x)}{dx} = nxP_n - nP_{n-1}(x) \tag{20}$$

If the order (m) is varying,

$$P_n^{m+1}(x) = \sqrt{x^2-1}[(n-m)xP_n^m(x) - (n+m)P_{n-1}^m(x)] \tag{21}$$

$$(x^2-1)\frac{dP_n^m(x)}{dx} = (n+m)(n-m+1)\sqrt{x^2-1}P_n^{m-1}(x) - mxP_n^m(x) \tag{22}$$

If the order (m) and the degree (n) are varying,

$$P_{n+1}^m(x) = P_{n-1}^m(x) + (2n+1)\sqrt{x^2-1}P_n^{m-1}(x) \tag{23}$$

It should also be noted that (A&S pg.333 8.4.1 and 8.4.3)

$$P_0^0(x) = 1 \tag{24}$$
$$P_1^0(x) = x \tag{25}$$

2. Orthonormality Test of the associated Legendre Polynomials A numerical test of the associated Legendre Polynomials tested can be performed using their orthonormality property. The normalized associated Legendre Polynomials are defined as:

$$\widetilde{P}_l^m(x) = \sqrt{\frac{(2l+1)}{2}\frac{(l-m)!}{(l+m)!}}P_l^m(x) \tag{26}$$

where

$$\{n|n \geq 0, n\epsilon\mathbb{Z}\}$$
$$\{m|m \geq 0, m\epsilon\mathbb{Z}\}$$
$$\{x|x\epsilon\mathbb{R}\}$$

and $P_l^m(x)$ are the non-normalized associated Legendre polynomials:

$$P_l^m(x) = (-1)^m \left(1-x^2\right)^{\frac{m}{2}} \frac{d^m}{dx^m} \left(P_l(x)\right) \tag{27}$$

where $P_l(x)$ are the Legendre Polynomials, expressed using Rodrigues' formula:

$$P_l(x) = \frac{1}{2^l l!} \frac{d^l}{dx^l} [\left(x^2-1\right)^l] \tag{28}$$

Now, orthonormality states that

$$\int_{-1}^{1} \widetilde{P}_l^m(x) \widetilde{P}_{l'}^m(x) dx = \delta_{ll'} \tag{29}$$

if $0 \le m \le l$ (taken from PN and `http://en.wikipedia.org/wiki/Associated_Legendre_polynomials`). Now, based on the Gauss-Legendre Quadrature

$$\int_{-1}^{1} \widetilde{P}_l^m(x) \widetilde{P}_{l'}^m(x) dx = \sum_{\alpha=1}^{n_\alpha} w_\alpha \widetilde{P}_l^m(x_\alpha) \widetilde{P}_{l'}^m(x_\alpha) = \delta_{ll'} \tag{30}$$

where the condition $l \le 2n-1$ is required for the relation to be exact (i.e. $R_n = 0$), as shown. The definitions of x_α and w_α can be found in section II B 1 a 3. If one defines a matrix,

$$L_{l\alpha}^m = \widetilde{P}_l^m(x_\alpha)\sqrt{w_\alpha} \tag{31}$$

then

$$\sum_{\alpha=1}^{n_\alpha} w_\alpha \widetilde{P}_l^m(x_\alpha) \widetilde{P}_{l'}^m(x_\alpha) = \sum_{\alpha=1}^{n} L_{l\alpha}^m (L_{l'\alpha}^m)^\intercal = \delta_{ll'} \tag{32}$$

thus

$$L^{n\intercal} L^m = L^n L^{m\intercal} = \mathbb{1} \tag{33}$$

I am not sure if the above is correct or if PN meant:

$$L^{l\intercal} L^{l'} = L^l L^{l'\intercal} = \mathbb{1} \tag{34}$$

Now, the $|lm\rangle$ is not a direct product of $|l\rangle$ and $|m\rangle$ (i.e. $|lm\rangle \neq |l\rangle\,|m\rangle$) as l and m are not independent quantum numbers, but $|m| \le l$, with the restriction that $l \ge 0$. This makes storing the $|lm\rangle$ basis in a matrix more difficult. However, this issue is at least partially alleviated by defining a new quantum number $n = l^2 + l + m$, with $0 \le n \le (l_{max}^2 + 2l_{max}) = (l_{max}+1)^2 - 1$.

3. Gauss-Legendre Quadrature From Abramowitz and Stegun pg.887, Section 25.4.29:
The quadrature is

$$\int_{-1}^{1} f(x) dx = \sum_{i=1}^{n} w_i f(x_i) + R_n \tag{35}$$

The related polynomials for this quadrature are the Legendre Polynomials $P_n(x)$. Also,

$$x_i = i\text{th root of } P_n(x) \tag{36}$$

$$w_i = \frac{2}{(1-x_i^2)(P_n'(x_i))^2} \tag{37}$$

$$R_n = \frac{2^{2n+1}(n!)^4}{(2n+1)[(2n)!]^3} f^{(2n)}(\xi), (-1 < \xi < 1) \tag{38}$$

It should be noted that $R_n = 0$ if $f(x)$ is a polynomial of degree $2n-1$ or less (as $f^{(2n)}(x) = 0$ in that case).

4. Gauss-Chebyshev Quadrature

b. Asymmetric Top

C. Potential Energy

1. Orientational

a. Linear Rotor Given a potential energy matrix $V(\theta,\phi)$ that is diagonal in θ and ϕ, V can be expressed as a vector $\vec{V}(\theta,\phi) = \mathrm{diag}(V)$.Now, the matrix elements of V are

$$V_{nn'}(\theta,\phi) = \int_0^{2\pi} \partial\phi \int_{-1}^{1} \partial(\cos\theta)\, Y_{lm[n]}(\theta,\phi)\, V(\theta,\phi)\, Y_{lm[n']}(\theta,\phi) \tag{39}$$

where $lm[n]$ denotes that the quantum numbers l and m are treated as a function of n. In this case, l and m are looked up in a table given n as the index. $Y_{lm[n]}(\theta,\phi)$ is defined as in (1) and (2), but is also defined here as

$$Y_{lm[n]}(\theta_\alpha,\phi_\beta) = P_{lm}(\cos\theta_\alpha)N_m(\phi_\beta) \tag{40}$$

where α and β are the indices of the θ and ϕ grids, respectively, such that $\theta\ \epsilon\ [0,\pi]$ and $\phi\ \epsilon\ [0,2\pi]$ so that

$$Y^{\alpha\beta}_{lm[n]} = P^{\alpha}_{lm[n]} N^{\beta}_{m[n]} \tag{41}$$

$$= P^{\alpha}_{lm} N^{\beta}_{m} \tag{42}$$

where the $lm[n]$ is changed to lm except where there is ambiguity in the index n.

Now, within the Lanczos algorithm, a Krylov subspace is generated using an initial vector $v_{n'}$ for the entire Hamiltonian. And, since, V is a part of the Hamiltonian, the potential Krylov vector is

$$u_n = \sum_{n'} V_{nn'} v_{n'} \tag{43}$$

Now, since both θ and ϕ are discretized, V can actually be calculated using a Gaussian Quadrature

$$V_{nn'} = \sum_{\alpha,\beta} Y^{\alpha\beta}_{lm[n]} w_\alpha^{\frac{1}{2}} w_\beta^{\frac{1}{2}} V_{\alpha\beta} w_\alpha^{\frac{1}{2}} w_\beta^{\frac{1}{2}} Y^{\alpha\beta}_{lm[n']} \tag{44}$$

where w_i are the weights for each grid and are split apart for the purposes of symmetric transformations. Thus,

$$u_n = \sum_{n'} V_{nn'} v_{n'} \tag{45}$$

$$= \sum_{n'} \sum_{\alpha,\beta} Y^{\alpha\beta}_{lm[n]} w_\alpha^{\frac{1}{2}} w_\beta^{\frac{1}{2}} V_{\alpha\beta} w_\alpha^{\frac{1}{2}} w_\beta^{\frac{1}{2}} Y^{\alpha\beta}_{lm[n']} v_{n'} \tag{46}$$

$$= \sum_{\alpha,\beta} Y^{\alpha\beta}_{lm[n]} w_\alpha^{\frac{1}{2}} w_\beta^{\frac{1}{2}} V_{\alpha\beta} w_\alpha^{\frac{1}{2}} w_\beta^{\frac{1}{2}} \sum_{n'} Y^{\alpha\beta}_{lm[n']} v_{n'} \tag{47}$$

2. Partial Summation

Similarly to the partial summation that can be performed for the direct product translational basis $|n_x n_y n_z\rangle$, it may be beneficial to try a partial summation method for the $|lm\rangle$ basis in order to have a computationally more efficient algorithm.

Now, the last sum in (47) can be broken apart and rearranged as follows

$$\sum_{n'} Y^{\alpha\beta}_{lm[n']} v_{n'} = \sum_{l=0}^{l_{max}} \sum_{m=-l}^{l} P^{\alpha}_{lm} N^{\beta}_{m} v_{lm} \tag{48}$$

$$= \sum_{m=-l_{max}}^{l_{max}} N^{\beta}_{m} \sum_{l=|m|}^{l_{max}} P^{\alpha}_{lm} v_{lm} \tag{49}$$

$$= \sum_{m=-l_{max}}^{l_{max}} N^{\beta}_{m} \tilde{v}^{\alpha}_{m} \tag{50}$$

where l_{max} is the highest l incorporated in the numerical calculations.

Now, though each of these forms has the same mathematical meaning, they may require a different number of FLOPS to actually be calculated. For (48), all of the terms are calculated at once within a double loop. The number of FLOPS for (48) is, however, twice the number of terms since the

For (49), both the outer and inner sums should be treated separately, hence equation (49). Concentrating on the inner sum, the number of terms is

$$\text{Terms}(\tilde{v}^{\alpha}_{m}) = \text{Terms}\left(\sum_{l=|m|}^{l_{max}} P^{\alpha}_{lm} v_{lm}\right) \tag{51}$$

$$= n_{\alpha}\left(l_{max} - |m| + 1\right) \tag{52}$$

where n_{α} is the number of α grid points.

However, this is not complete. For when $\tilde{v}^{\alpha}_{m}$ is calculated, one must also perform the calculation for all of the m terms within the vector, since P^{α}_{lm} also depends on m. Thus, the number of terms is

$$\text{Terms}(\tilde{v}^{\alpha}_{m}) = \sum_{m=-l_{max}}^{l_{max}} \text{Terms}\left(\sum_{l=|m|}^{l_{max}} P^{\alpha}_{lm} v_{lm}\right) \tag{53}$$

$$= \sum_{m=-l_{max}}^{l_{max}} n_{\alpha}\left(l_{max} - |m| + 1\right) \tag{54}$$

$$= n_{\alpha} \sum_{m=-l_{max}}^{l_{max}} \left(l_{max} - |m| + 1\right) \tag{55}$$

$$= n_{\alpha}\left(2\sum_{m=1}^{l_{max}} \left(l_{max} - m + 1\right) + \left(l_{max} - |m| + 1\right)_{m=0}\right) \tag{56}$$

$$= n_{\alpha}\left(2\left(\sum_{m=1}^{l_{max}} l_{max} - \sum_{m=1}^{l_{max}} m + \sum_{m=1}^{l_{max}} 1\right) + l_{max} + 1\right) \tag{57}$$

$$= n_{\alpha}\left(2\left(l_{max}^2 - \frac{l_{max}\left(l_{max}+1\right)}{2} + l_{max}\right) + l_{max} + 1\right) \tag{58}$$

$$= n_{\alpha}\left(2l_{max}^2 - l_{max}^2 - l_{max} + 2l_{max} + l_{max} + 1\right) \tag{59}$$

$$= n_{\alpha}\left(l_{max}^2 + 2l_{max} + 1\right) \tag{60}$$

$$= n_{\alpha}\left(l_{max} + 1\right)^2 \tag{61}$$

Thus, there are $n_{\alpha}\left(l_{max}+1\right)^2$ multiplications required (i.e. FLOPS) in order to calculate $\tilde{v}^{\alpha}_{m}$. From this point, one then needs to calculate $\sum_{m=-l_{max}}^{l_{max}} N^{\beta}_{m} \tilde{v}^{\alpha}_{m}$, which has the number of terms

$$\text{Terms}\left(\sum_{m=-l_{max}}^{l_{max}} N^{\beta}_{m} \tilde{v}^{\alpha}_{m}\right) = n_{\alpha} n_{\beta}\left(2l_{max} + 1\right) \tag{62}$$

where n_β is the number of grid points for the β basis. Now, similar to the reasoning that the calculation of $\tilde{v}_m^\alpha$ must include the calculation of all m terms, so here, since $\tilde{v}_m^\alpha$ is dependent on α, does $\sum_{m=-l_{max}}^{l_{max}} N_m^\beta \tilde{v}_m^\alpha$ need to include all α terms.

This leaves the total number of terms as

$$\mathrm{Terms}\left(\sum_{n'} Y_{lm[n']}^{\alpha\beta} v_{n'}\right) = \mathrm{Terms}\left(\sum_{m=-l_{max}}^{l_{max}} N_m^\beta \tilde{v}_m^\alpha\right) + \mathrm{Terms}(\tilde{v}_m^\alpha) \tag{63}$$

$$= n_\alpha \left(l_{max}+1\right)^2 + n_\alpha n_\beta \left(2l_{max}+1\right) \tag{64}$$

$$= n_\alpha [\left(l_{max}+1\right)^2 + n_\beta \left(2l_{max}+1\right)] \tag{65}$$

Here, it can be seen that though the α grid must be iterated through for the whole calculation, the β grid need only be evaluated for the $2l_{max}+1$ terms. This may give a potential computational cost savings.