# What this code is about

The C++ code moments.cpp computes the Rayleigh-Schrodinger perturbation expansion coefficients $E^{(2k)}$

$$E_0(\beta) = 1 + \sum_{k=1}^{\infty} E^{(2k)}(-\beta)^k \tag{1}$$

for the ground-state energy of the $\mathcal{P} - \mathcal{T}$ symmetric cubic oscillator. We use the following formulae,

$$E^{(2k)} = \frac{3}{\sqrt{8}} a_{0,1}^{(2k-1)} + \frac{\sqrt{6}}{\sqrt{8}} a_{0,3}^{(2k-1)}, \qquad E^{(2k+1)} = 0 \tag{2}$$

where

$$a_{0,1}^{(2k-1)} = -\frac{1}{2} \left( \langle 1|x^3|2 \rangle \, a_{0,2}^{(2k-2)} + \langle 1|x^3|4 \rangle \, a_{0,4}^{(2k-2)} - \sum_{s=1}^{2k-2} a_{0,1}^{(s)} E^{(2k-2-s)} \right) \tag{3}$$

and

$$a_{0,3}^{(2k-1)} = -\frac{1}{6} \left( \langle 3|x^3|2 \rangle \, a_{0,2}^{(2k-2)} + \langle 3|x^3|4 \rangle \, a_{0,4}^{(2k-2)} + \langle 3|x^3|6 \rangle \, a_{0,6}^{(2k-2)} \right.$$
$$\left. - \sum_{s=1}^{2k-2} a_{0,3}^{(s)} E^{(2k-2-s)} \right) \tag{4}$$

and in general,

$$a_{0,m}^{(r)} = -\frac{1}{2m} \left( \langle m|x^3|m-3 \rangle \, a_{0,m-3}^{(r-1)} + \langle m|x^3|m-1 \rangle \, a_{0,m-1}^{(r-1)} \right. \tag{5}$$
$$+ \langle m|x^3|m+1 \rangle \, a_{0,m+1}^{(r-1)} + \langle m|x^3|m+3 \rangle \, a_{0,m+3}^{(r-1)} \tag{6}$$
$$\left. - \sum_{s=1}^{r-1} a_{0,m}^{(s)} E^{(r-s)} \right), \qquad r \geq 2 \tag{7}$$

The non-zero matrix elements

$$\langle n|x^3|n+3\rangle = \frac{1}{\sqrt{8}}\sqrt{(n+3)(n+2)(n+1)} \tag{8}$$

$$\langle n|x^3|n+1\rangle = \frac{3}{\sqrt{8}}(n+1)\sqrt{n+1} \tag{9}$$

$$\langle n|x^3|n-1\rangle = \frac{3}{\sqrt{8}}(n)\sqrt{n} \tag{10}$$

$$\langle n|x^3|n-3\rangle = \frac{1}{\sqrt{8}}\sqrt{(n-2)(n-1)n}. \tag{11}$$

The coefficients $E^{(2k)}$ are written to the file moments.txt.

The file compile.job is a SLURM script to compile the code in an HPC and generate an executable.

The file together.job is a SLURM script to run the executable in an HPC.

The file mpfr.sh is a shell script used to compile and run the code in an Ubuntu 22.04 local machine.