What this code is about

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

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

for the ground-state energy of the quartic anharmonic oscillator. We computed up to $k = d, d-1, ..., 1$ recursively using the following formulae,

$$b^{(k)} = \frac{3\sqrt{2}}{3}\, a_{0,2}^{(k-1)} + \frac{\sqrt{6}}{2}\, a_{0,4}^{(k-1)}, \qquad k \geq 2 \tag{2}$$

with

$$b^{(0)} = 1 \qquad \text{and} \qquad b^{(1)} = \frac{3}{4}, \tag{3}$$

and

$$\begin{aligned} a_{0,2}^{(k-1)} = -\frac{1}{4} \Big(& \langle 2|x^4|2\rangle\, a_{0,2}^{(k-2)} + \langle 2|x^4|4\rangle\, a_{0,4}^{(k-2)} \\ & + \langle 2|x^4|6\rangle\, a_{0,6}^{(k-2)} - \sum_{s=1}^{k-2} a_{0,2}^{(s)}\, b^{(k-1-s)} \Big), \end{aligned} \tag{4}$$

$$a_{0,2}^{(1)} = -\frac{\langle 2|x^4|0\rangle}{4}, \tag{5}$$

$$\begin{aligned} a_{0,4}^{(k-1)} = -\frac{1}{8} \Big(& \langle 4|x^4|2\rangle\, a_{0,2}^{(k-2)} + \langle 4|x^4|4\rangle\, a_{0,4}^{(k-2)} \\ & + \langle 4|x^4|6\rangle\, a_{0,6}^{(k-2)} + \langle 4|x^4|8\rangle\, a_{0,8}^{(k-2)} - \sum_{s=1}^{k-2} a_{0,4}^{(s)}\, b^{(k-1-s)} \Big), \end{aligned} \tag{6}$$

$$a_{0,4}^{(1)} = -\frac{\langle 4|x^4|0\rangle}{8}. \tag{7}$$

and in general,

$$a_{0,m}^{(1)} = -\frac{\langle m|x^4|0\rangle}{2m} \tag{8}$$

$$a_{0,m}^{(r)} = -\frac{1}{2m}\left(\sum_{k=1}^{\infty}\langle m|x^4|k\rangle\, a_{0,k}^{(r-1)} - \sum_{s=1}^{k-1} a_{0,m}^{(s)}\, b^{(r-s)}\right), r \geq 2,\ m \neq 0,$$

the infinite sum becomes finite since the following are the only non-zero matrix elements,

$$\langle n|x^4|n+4\rangle = \frac{1}{4}\sqrt{(n+1)(n+2)(n+3)(n+4)} \tag{9}$$

$$\langle n|x^4|n+2\rangle = \frac{1}{2}(2n+3)\sqrt{(n+1)(n+2)} \tag{10}$$

$$\langle n|x^4|n\rangle = \frac{3}{2}\left(n^2+n+\frac{1}{2}\right) \tag{11}$$

$$\langle n|x^4|n-2\rangle = \frac{1}{2}(2n-1)\sqrt{n(n-1)} \tag{12}$$

$$\langle n|x^4|n-4\rangle = \frac{1}{4}\sqrt{n(n-1)(n-2)(n-3)} \tag{13}$$

The coefficients b^k 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.