Question regarding ALPS fulldiag

Dear ALPS Developers,

I am getting unexpected results using the ALPS fulldiag application and I would be glad if you could give me some feedback as to whether the observed behavior is intended or not.

I have tracked-down the problem to the following simple test case, using ALPS 2.2.b3 on Euler (compiled using GCC and threaded Intel MKL). The test case consists of a spin-ladder with 4 unit cells, and should be reproducible using the attached Python script *fulldiag_run.py*. The only two parameters I am tweaking in the following are *TRANSLATION_SYMMETRY* and *COMPLEX*. To simplify things, I solve the model on the $S_z^{\text{tot}} = -1$ sector only. The relevant measurements for the following discussion are energy and average S_z ("*Szavg*").

- When I run the calculation with *TRANSLATION_SYMMETRY*=*COMPLEX*=False, I obtain a reasonably-looking spectrum and the average S_z is $\approx -\frac{1}{8}$.[1]
- When I switch to *TRANSLATION_SYMMETRY*=*COMPLEX*=True, the energies reported for sector 1 ($k = \frac{\pi}{2}$), are a subset of those obtained without using translation symmetry, i. e. consistent. The average S_z values however, are far from the expected value $-\frac{1}{8}$.[2]
- For completeness, I have tried setting *TRANSLATION_SYMMETRY*=True and *COMPLEX*=False. Since a basis, which diagonalizes the tranlation operators should contain complex phase factors, I do not expect this to work. Indeed, I get energies which do not occur in the spectrum calculated without translation symmetry, cf. $k = \frac{\pi}{2}$ sector again. Nonetheless, this time the average S_z looks "correct".[3]

To summarize, my problem is that the correlators and average measurements seem strange when making use of translation-symmetry. Any input on the this issue would be highly appreciated.

[1] Output data file test_L4_Sz_Sz1.task1.out.h5
[2] Output data file test_L4_k_Sz_cmplx_Sz1.task1.out.h5
[3] Output data file test_L4_k_Sz_Sz1.task1.out.h5