Report on CPD based Coupled Cluster

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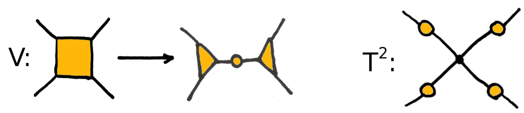
1 Description

As was shown earlier, Coupled Cluster can be solved approximately by imposing some tensor decomposition with low number of parameters on cluster amplitudes. By combining this with an approximation of the Hamiltonian and the "energy denominator" tensors one can produce variants of Coupled Cluster theory with low scaling. In these notes the results for Canonical Decomposition of amplitudes, RI decomposition of the two electron integrals and canonical decomposition of energy denominator are listed. As a reminder, RI and CPD decompositions are defined as

$$V_{ijkl} = \sum_{pq}^{R_v} W^1_{ijp} \cdot S_{pq} \cdot W^2_{qkl} \tag{1}$$

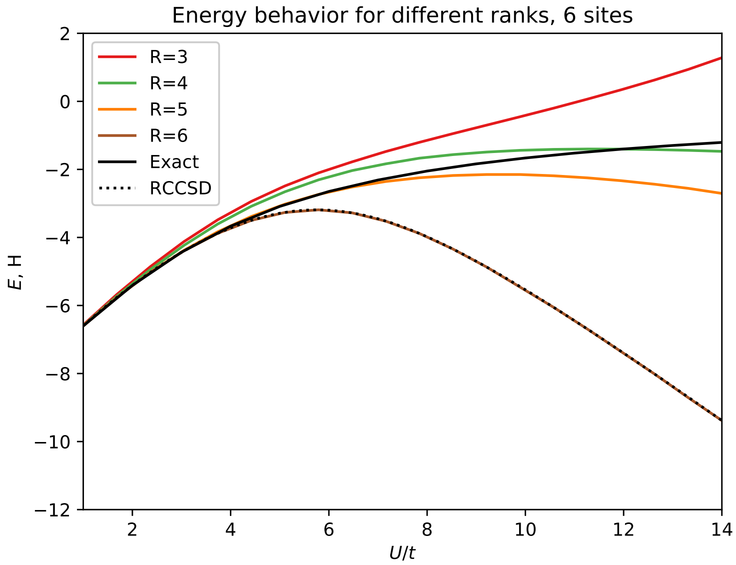
$$T^2_{ijab} = \sum_{t}^{R_t} X^1_{it} \cdot X^2_{jt} \cdot X^3_{at} \cdot X^4_{bt} \tag{2}$$

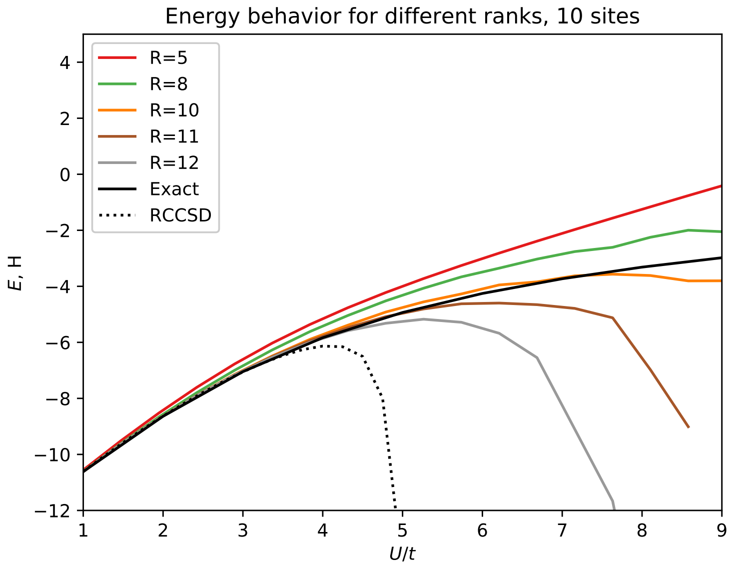


To estimate the norm of each rank-1 tensor in the CPD, I sligthly modified CPD decomposition of T^2 and forced the columns of X^n to have unit norms. The normalized decomposition is defined as

$$T^2_{ijab} = \sum_{t}^{R_t} \Lambda_t X^1_{it} \cdot X^2_{jt} \cdot X^3_{at} \cdot X^4_{bt} \tag{3}$$

where Λ is a vector containing weights of the normalized factors. The new decomposition is denoted as nCPD, and seems to have almost identical properties to the original one. All discussed Coupled Cluster codes were derived both for CPD and nCPD decomposed amplitudes.

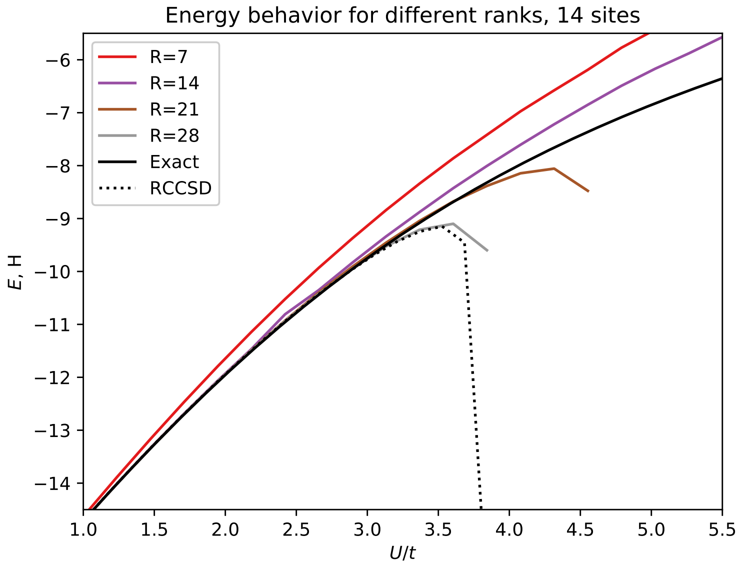


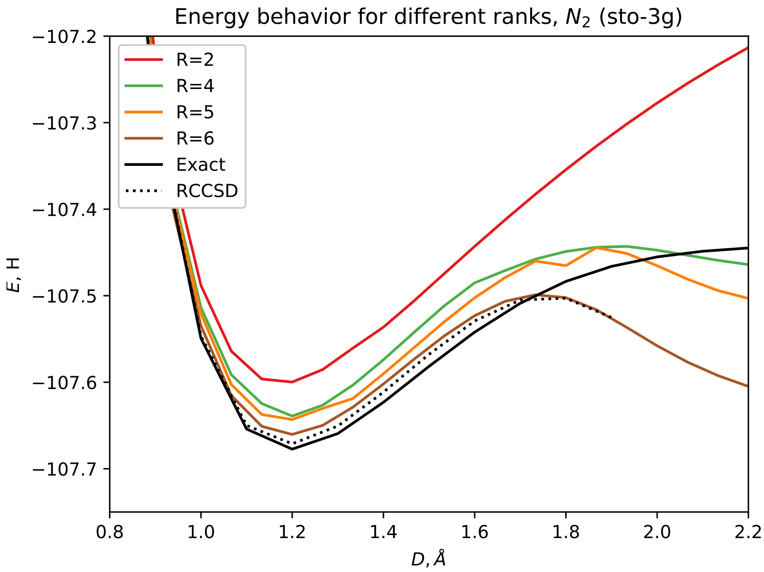


2 Approximation properties

Let us start with the discussion of the RCCSD-CPD. Energy behavior versus the rank of CPD for various systems is shown below.

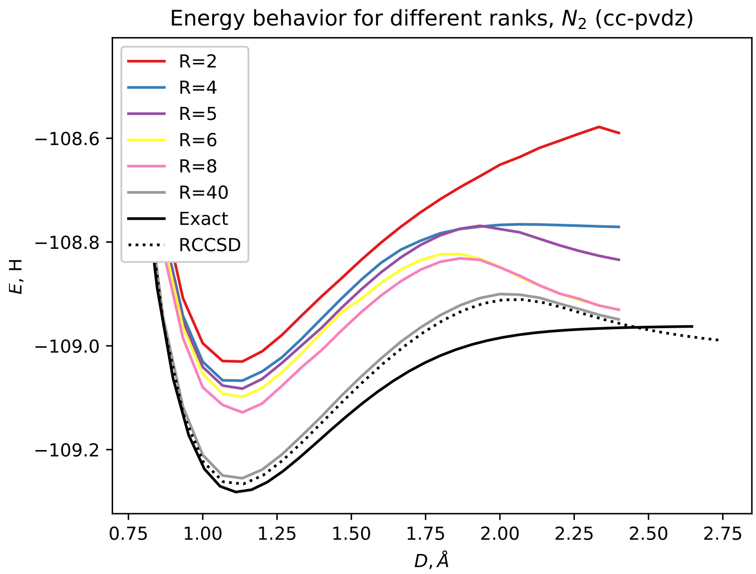
The performance of the method has distinct features in two regimes: weak and strong correlation. In weak correlation regime the errors are small. In strong correlation regime the difference between approximate and regular Coupled Cluster may be large, but approximate solutions have better behavior com-





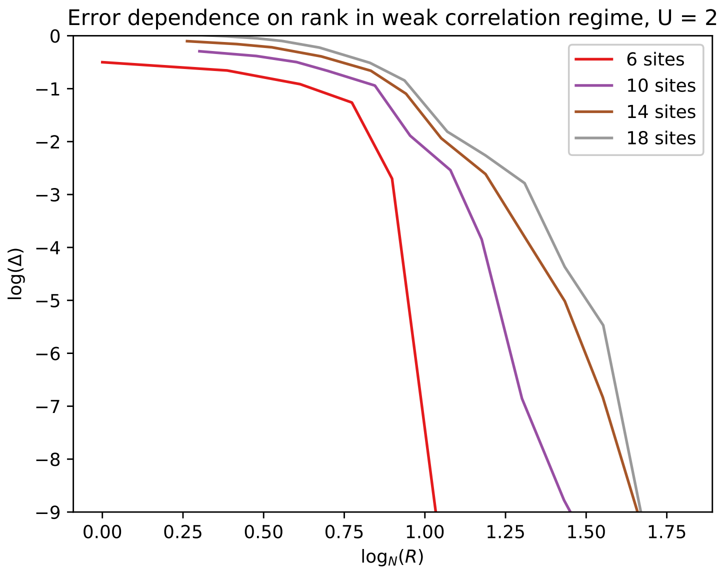
pared to regular ones.

We have to note that the method is not convergent for large ranks at strong correlation. Normal Coupled Cluster is also non convergent by naive iterations unless damping or DIIS is used. I have not found a robust way to do DIIS in the current implementation. This aspect needs more thinking and experimentation. Additionally, CC methods with decomposed amplitudes may require a lot a iterations to converge.



3 Weak correlation

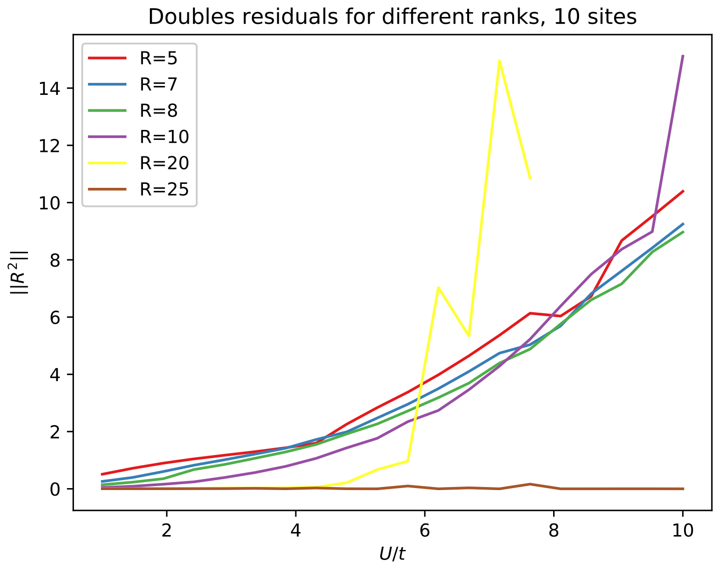
Let us estimate how well the approximation works in the weak correlation case.



For weak correlation the difference in the energy between RCCSD-CPD and classical RCCSD decays exponentially with respect to the decomposition rank, which is less than N^2. We have to note that a fixed $U = 2$ does not set an equivalent correlation strength for tested Hubbard models.

4 Strong correlation

It's interesting to note that in strong correlation limit very low rank decompositions seem to generate solutions with good physical behavior. Let us look at other parameters of Coupled Cluster in this regime. We consider a 10-site Hubbard with PBC at $U = 2$.



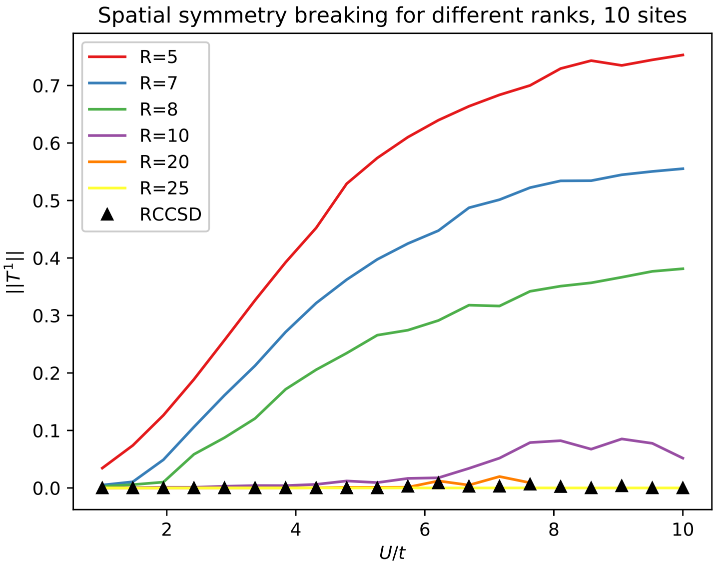
Decomposed amplitudes are not exact solutions of CC equations. As correlation strength grows doubles residuals of RCCSD-CPD increase (and equations are getting progressively harder to converge). As the rank grows those residuals decrease, because decomposed solutions are becoming better approximations to the conventional CC amplitudes, where all residuals are zero.

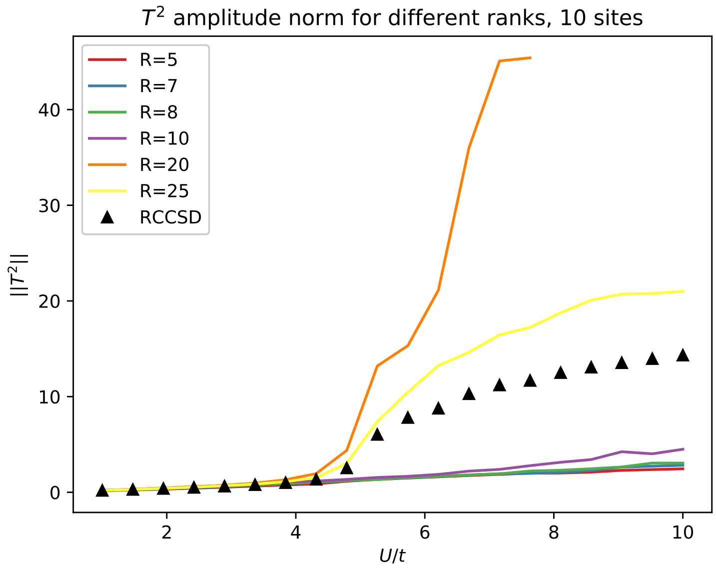
T^1 amplitudes are, however, true solutions to CC equations, because we do not approximate them. This results in T^1 amplitudes becoming non-zero at convergence as they adapt to approximate low-norm T^2, while they should be zero for Hubbard models due to symmetry. As the rank of the decomposition increases T^1 amplitudes go to their expected values (zero).

Let us look at the norm of T^2. As was found in PoST and Attenuated-CC works, the cause of the bad performance of Coupled cluster in strong correlation regime is the growth of higher order CC amplitudes. It turns out that low rank structure of T^2 has an effect of regularization. As the rank increases, T^2 amplitudes are getting less regularized and approach their conventional values, which are high.

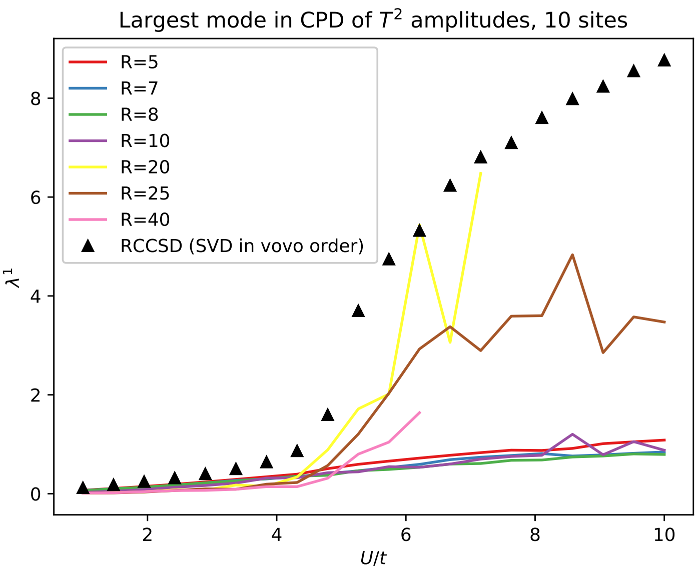
Finally, let us look at the norms of individual components of T^2 amplitudes, as we keep them in the normalized form (RCCSD-nCPD). The first component follows closely the total norm of amplitudes.

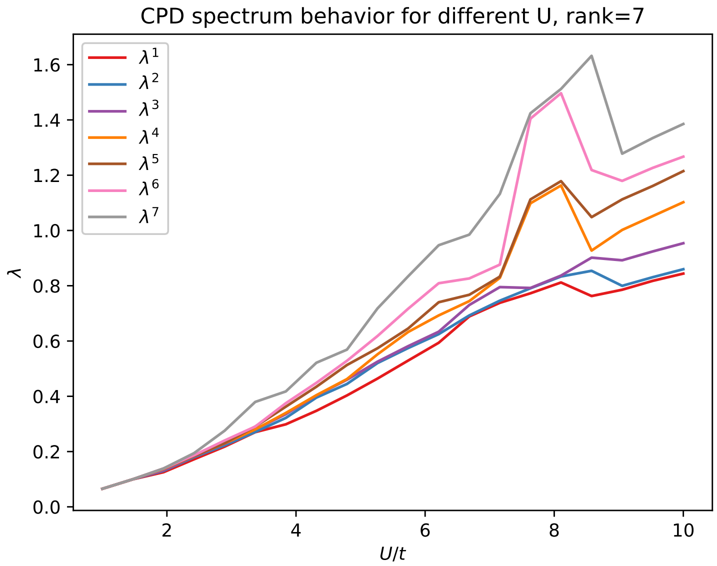
The full spectrum, however, does not have a distinct dominant mode neither in low nor in large rank regime. This contrasts with the case of SVD in regular Coupled Cluster, where the broken symmetry mode is clearly seen. For CPD this is not the case, possibly because the individual components of CPD are

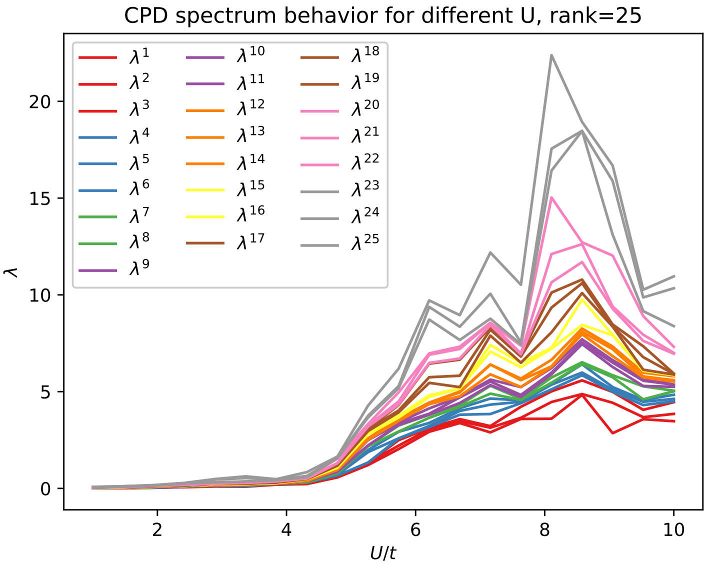


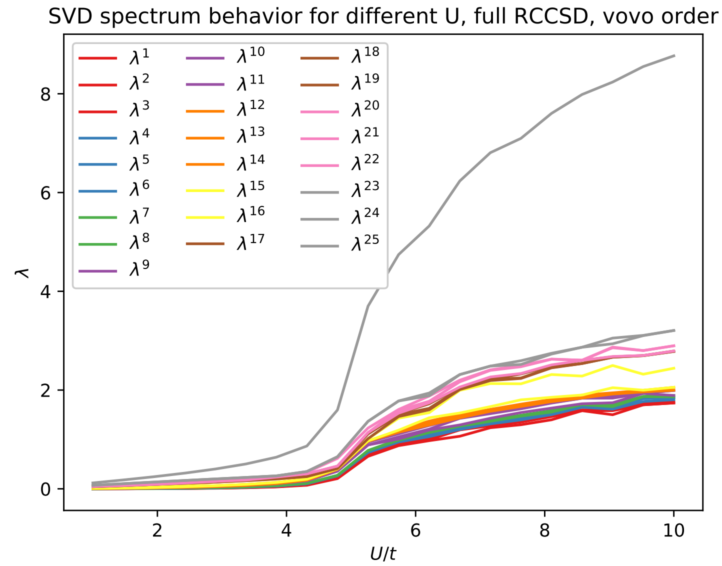


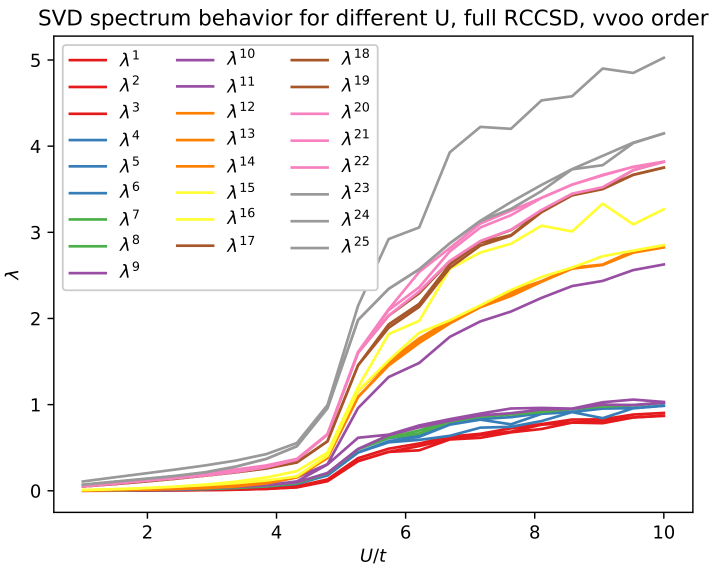
not orthogonal to each other. Solving this issue (by imposing some additional constraint on the structure of T^2) will provide a direct way to Attenuated CC with decomposed amplitudes.


Largest mode in CPD of T^2 amplitudes, 10 sites
R=5
R=7
R=8
R=10
R=20
R=25
R=40
RCCSD (SVD in vovo order)
λ^1
U/t


CPD spectrum behavior for different U, rank=7
λ^1
λ^2
λ^3
λ^4
λ^5
λ^6
λ^7
λ
U/t


CPD spectrum behavior for different U, rank=25
λ^1
λ^2
λ^3
λ^4
λ^5
λ^6
λ^7
λ^8
λ^9
λ^{10}
λ^{11}
λ^{12}
λ^{13}
λ^{14}
λ^{15}
λ^{16}
λ^{17}
λ^{18}
λ^{19}
λ^{20}
λ^{21}
λ^{22}
λ^{23}
λ^{24}
λ^{25}
λ
U/t


SVD spectrum behavior for different U, full RCCSD, vovo order
λ^1
λ^2
λ^3
λ^4
λ^5
λ^6
λ^7
λ^8
λ^9
λ^{10}
λ^{11}
λ^{12}
λ^{13}
λ^{14}
λ^{15}
λ^{16}
λ^{17}
λ^{18}
λ^{19}
λ^{20}
λ^{21}
λ^{22}
λ^{23}
λ^{24}
λ^{25}
λ
U/t


SVD spectrum behavior for different U, full RCCSD, vvoo order
λ
U/t
λ1
λ2
λ3
λ4
λ5
λ6
λ7
λ8
λ9
λ10
λ11
λ12
λ13
λ14
λ15
λ16
λ17
λ18
λ19
λ20
λ21
λ22
λ23
λ24
λ25
0
1
2
3
4
5
2
4
6
8
10