**Table 3.** Summary of internal tolerances in *Spinach*

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| **Tolerance** | **Default Value** | **Comments** |
| sys.tols.liouv\_zero | 1×10–7 | Elements of the Liouvillian with absolute values below this threshold are set to zero and dropped from the sparse array. |
| sys.tols.rlx\_zero | 1×10–7 | Elements of the relaxation superoperator with absolute values below this threshold are set to zero and dropped from the sparse array. |
| sys.tols.prop\_zero | 1×10–8 | Elements of the exponential propagator with absolute values below this threshold are set to zero and dropped from the sparse array. |
| sys.tols.prop\_norm | 1×10–9 | If the exponential propagator is generated using a series expansion, the contributions from terms with infinity-norm smaller than this tolerance are ignored. |
| sys.tols.prop\_chop | 1×10–10 | If the exponential propagator is generated using a series expansion, the elements of the series terms with absolute values below this threshold are set to zero and dropped from the sparse array. |
| sys.tols.derivative\_prop\_zero | 1×10–8 | Elements of the derivative propagator with absolute values below this threshold are set to zero and dropped from the sparse array. |
| sys.tols.derivative\_prop\_norm | 1×10–9 | If a derivative propagator is generated using a series expansion, the contributions from terms with infinity-norm smaller than this tolerance are ignored. |
| sys.tols.derivative\_prop\_chop | 1×10–10 | If a derivative propagator is generated using a series expansion, the elements of the series terms with absolute values below this threshold are set to zero and dropped from the sparse array. |
| sys.tols.krylov\_dim | 30 | Maximum Krylov subspace dimension for Krylov propagation using expv. |
| sys.tols.krylov\_tol | 1×10–7 | Krylov subspace orthogonality tolerance for Krylov propagation using expv. |
| sys.tols.krylov\_switchover | 50000 | The number of non-zeros in the Liouvillian, above which the Krylov propagation method would be used. |
| sys.tols.zte\_tol | 1×10–30 | In the Zero Track Elimination procedure, any states yielding tracks with infinity-norm below this threshold are dropped from the basis. |
| sys.tols.zte\_nsteps | 10 | The number of time steps in the trajectory used to identify zero tracks. The time step is set automatically to . |
| sys.tols.zte\_maxden | 0.5 | The fraction of non-zeros in the state vector, above which the ZTE procedure would be skipped automatically. |
| sys.tols.prox\_cutoff | 4 | Dipolar interaction for a pair of spins at a separation (in Ångstrom) greater than this threshold is set to zero. |
| sys.tols.inter\_cutoff | 1×10–5 | If the 2-norm of an interaction tensor is below this threshold, the interaction is ignored. |
| sys.tols.basis\_hush | 256 | If the number of vectors in the basis is above this threshold the full state list is not printed to the log. |
| sys.tols.inter\_sym | 1×10–5 | If the 2-norm of the anti-symmetric part of an interaction tensor is smaller than this parameter, the tensor is symmetrised to machine precision. |
| sys.tols.path\_trace | 1×10–7 | If a Liouvillian element is found to be smaller than this threshold, the element is ignored in the path tracing procedure. |
| sys.tols.path\_drop | 1×10–10 | If the 2-norm of the state vector projection into an independently evolving subspace is found to be smaller than this threshold, the subspace is dropped from the simulation. |
| sys.tols.irrep\_drop | 1×10–10 | If the 2-norm of the state vector projection into an irreducible representation of the symmetry group is found to be smaller than this threshold, the irrep is dropped from the simulation. |
| sys.tols.small\_matrix | 200 | If a matrix is found to be smaller than this threshold dense algebra is used. |
| sys.tols.dense\_matrix | 0.25 | If the fraction of non-zeros in a matrix is found to be greater than this threshold, dense matrix algebra is used. |
| sys.tols.rlx\_integration | 1×10–4 | Relative accuracy of numerical integration in the evaluation of Redfield superoperator. |
| sys.tols.grid\_rank | 131 | The rank of the Lebedev grid used for orientational averaging. |
| sys.tols.dP\_method | ‘hausdorff’ | A switch controlling the selection of the exponential propagator differentiation method. The finite-difference method (‘finite-difference’) uses the second-order central method with an automatically determined stepping. |
| sys.tols.dP\_order | Inf | The order at which the Hausdorff series is to be terminated during the calculation of propagator derivatives if the accuracy goal has not been achieved yet. |
| sys.tols.normest\_tol | 5×10–4 | Matrix norm estimation tolerance for the stages where quick matrix norm estimates using *normest* are employed. |
| sys.tols.exponentiation | ‘taylor’ | A switch controlling the selection of sparse matrix exponentiation procedure – either scaled Taylor series or scaled Chebyshev (‘chebyshev’) series. |