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        Diffusion Along a Circle
        (Canonical Ensemble)
        Eigensystem Approach

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COMMAND LINE SYNTAX:

DIFF initial_state_pattern output_file [options]

initial_state_pattern ... A character sequence that encodes a valid pattern of atoms,
                          serving as the initial state of the system.  Valid patterns
                          consist of the characters "o" (sites occupied by atoms) and
                          "." (empty sites).  The total number of sites p (i.e., the
                          length of the character sequence) must be a prime number
                          between 3 and 31.

output_file ............. The path and file name for the output files, without file
                          extensions.  DIFF will normally create two output files,
                          output_file.INF (a file containing information on the
                          decomposition into eigenstates), and output_file.DAT (a file
                          displaying the temporal evolution of pattern averages).

OPTIONS ................. The following optional switches control the execution of DIFF.
                          (They must be separated by blanks.)

/? ...................... Display a short overview of the DIFF command line options.

/1 ...................... Calculate temporal evolution data for all p single-site
                          averages [default]

/2 ...................... Calculate temporal evolution data for all two-site atom-atom
                          correlators, i.e., the probability to find two atoms at each
                          pair of pre-specified sites.

/A=rate ................. Rate for atomic jumps of type "A" (atomic jumps without
                          initial or final neighbour) [default value: 1.0]

/B=rate ................. Rate for atomic jumps of type "B" (atomic jumps with
                          initial, but without final neighbour) [default value: 1.0]

/c[heck] ................ Check accuracy of numerical diagonalization scheme.  If
                          activated, DIFF provides information about the numerical
                          deviations incurred in the spectral decomposition of
                          unity and the symmetrized rate matrices (L2 or Schur norm).
                          This option significantly increases execution time and is
                          provided for testing purposes.

/C=rate ................. Rate for atomic jumps of type "C" (atomic jumps without
                          initial, but with final neighbour) [default value: 1.0]

/d=digits ............... Numerical precision of evolution data output in digits.
                          Allowed values are 2 ... 16 [default: 6]

/D=rate ................. Rate for atomic jumps of type "D" (atomic jumps with both
                          initial and final neighbours) [default value: 1.0]

/e[igenvalues] .......... Force output of ordered eigenvalue list of rate coefficient
                          matrix for each momentum q = 0,1,...,(p-1)/2.

/E[igenvectors] ......... Supply eigenvectors of symmetrized rate coefficent matrix.
                          This switch must be combined with /e to take effect.
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                        Note:  The size of the output can be very significant, and
                        the option is mainly provided for testing purposes.

/h[elp] ................. Display a short overview of the DIFF command line options.

/l=block_data_file ...... Load decomposition of transformation matrix from disk.
                        (The extension .BLK will be appended to block_data_file.)
                        The data must have been saved to disk before using the /s
                        option.  The stored parameter set is checked for
                        compatibility.  This option provides the opportunity to
                        speed up serial computations that employ the same number
                        of sites, atoms, and identical rate parameters.

/L[og time scale] ....... Use a logarithmic time scale in the generation of temporal
                        evolution data [default: linear].

/n[o temporal evolution]  Suppress output of temporal evolution data.  Only information
                        on the diagonalization procedure and equilibrium averages (if
                        selected using the /q switch) will be produced.

/o[utput rate matrix] ... Supply the rate coefficent matrix in symbolic form.  The data
                        will consist of three parts:  A rate matrix for forward
                        (clockwise) jumps, a rate matrix for backward (counterclock-
                        wise) jumps, and the loss terms for each site (diagonal
                        entries).  Note:  The output can be substantial in size.

/p[rimitives] ........... Display all primitive patterns, i.e., all significantly (apart
                        from rotations) different arrangements of the atoms on the p
                        sites.  The option also provides information on the mirror
                        symmetry properties of the patterns.

/P=pattern .............. Provide temporal evolution of average of specified pattern(s).
                        Valid patterns consist of p symbols (p - number of sites) and
                        are composed of the tokens "o" (atom occupies designated site),
                        "." (site is empty), and "x" (content of site not specified).
                        The /P option may occur up to 512 times in the command line,
                        facilitating simultaneous evaluation of multiple patterns.

/q[uilibrium averages] .. Output equilibrium average for selected pattern(s).

/s=block_data_file ...... Save decomposition of transformation matrix to disk.  (The
                        extension .BLK will be appended to block_data_file.)  In
                        later runs, the data can be read from disk using the /l option,
                        allowing to speed up serial computations that share the same
                        number of sites and atoms, and employ identical jump rates.

/S=steps ................ Number of time steps used in the evaluation of temporal
                        averages [default value: 100]

/t=start_time ........... Initial time for calculation of temporal averages
                        [default value: 0.0]

/T=stop_time ............ Final time for calculation of temporal averages
                        [default value: 10.0]

/u[nitary trafo skip] ... Calculate and output eigenvalues only, but skip evaluation
                        of unitary transform.  With this option, the eigenvectors
                        remain undefined, and no temporal evolution data will be
                        produced.  This option speeds up execution time
                        considerably, and drastically reduces memory requirements.
                        It is incompatible with the options /c (accuracy check),
                        /E (eigenvector output) and /s (save block data), however.

/v[ariation from eqlib] . Generate temporal evolution data output that contains the
                        deviation from the equilibrium average of the selected
                        pattern(s) rather than their actual average occupation.
                        This option automatically activates the output of the
                        corresponding equilibrium averages (the /q option).
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/x[ponential format] .... Force temporal evolution data output in scientific notation (mantissa-exponent format), instead of the default fixed width notation. (The number of significant digits is controlled by the /d option.)

/y[mmetrize vectors] .... Post-symmetrize eigenvectors of the q=0 momentum subspace. This option enforces projection of the numerically determined eigenvectors on the symmetric and antisymmetric subspaces with respect to mirror reflection. Its usage will resolve the degeneracy of eigenvalues that occurs for identical jump rate parameters. However, it introduces an additional numerical error into the diagonalization scheme that can be significant if two eigenvalues in the same subspace are almost degenerate. The evaluation of the eigenvalues itself is not affected.

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REMARK ON COMMAND LINE LIMITS

Under MS-DOS, the length of a single command line is limited to 126 characters. This presents a severe limitation of the functionality of the DIFF command, since a large number of options is available. In particular, the problem affects multiple custom comparison patterns specified using the /P option which occupy (p + 4) characters per pattern, and easily extend the command line beyond the 126 character limit.

To work around this problem under MS-DOS, several strategies are available:

(i) Compilation using the Microsoft Visual C++ compiler. The executables thus generated apparently do not obey the 126 byte limit, but read options past this boundary.

(ii) The response file method. For programs created with the GNU gcc compiler (and possibly others), there is an option to redirect the input at run time: Instead of reading from the command line, DIFF reads the program arguments from a file. Up to 16 kByte of text can be supplied to DIFF using this method. It works as follows:

(a) Store the arguments and options chosen for the DIFF run in a file, say OPTIONS.OPT. This is the response file.

(b) Run DIFF from the command line or a batch file, but use the name of the response file as the argument, preceded by the special character @:

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DIFF @OPTIONS.OPT
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Then, the contents of OPTIONS.OPT will provide the remainder of the command line, i.e., the arguments and options supplied to DIFF.

For more information, see the DJGPP documentation.