# Structure of the wavefunction array

## 1 The MCTDH wavefunction

The standard MCTDH wavefunction can be written either in the multi-set

$$\Psi(\boldsymbol{q},t) = \sum_{s=1}^{n_s} \sum_{j_1^s \dots j_f^s}^{N} A_{j_1^s \dots j_f^s}(t) \varphi^{(\kappa)}_{j_1^s}(q_1,t) \cdots \varphi^{(\kappa)}_{j_f^s}(q_f,t)$$

or single-set formalism

$$\Psi(\boldsymbol{q},t) = \sum_{j_1 \dots j_f, s}^{N} A_{j_1 \dots j_f, s}(t) \varphi^{(\kappa)}_{j_1}(q_1) \cdots \varphi^{(\kappa)}_{j_f}(q_f) |s\rangle$$

In Quantics the wavefunction is stored in the `psi` array and the different parts accessed by pointers. How the pointers can be used to unfold the wavefunction is shown in Fig. 1. The Analyse programs `rdacoeff` and `rdspfs` can be used to extract and write the A-coefficients and SPFs to ascii files. The structure of this data is described below.

### 1.1 The A-vector

The A-coefficients are stored as a vector, or in the multi-set formalism a set of vectors. The vector indices, $J$,

$$A_J = A_{j_1 \dots j_f}$$

are a multi-index that can be related to the mode indices by raising the mode indices in sequence. The program `rdacoeff` simply writes the vector and the multi-index $J$.

As an example, for a 3D system that has 3 SPFs for each mode, there are 27 configurations and the indices are related as shown in Table 1

Table 1: The A-vector indices for a 3D system with 3 SPFs per mode

| vector index | Mode indices | | | vector index | Mode indices | | | vector index | Mode indices | | |
|---|---|---|---|---|---|---|---|---|---|---|---|
| $J$ | $j_1$ | $j_2$ | $j_3$ | $J$ | $j_1$ | $j_2$ | $j_3$ | $J$ | $j_1$ | $j_2$ | $j_3$ |
| 1 | 1 | 1 | 1 | 10 | 1 | 1 | 2 | 19 | 1 | 1 | 3 |
| 2 | 2 | 1 | 1 | 11 | 2 | 1 | 2 | 20 | 2 | 1 | 3 |
| 3 | 3 | 1 | 1 | 12 | 3 | 1 | 2 | 21 | 3 | 1 | 3 |
| 4 | 1 | 2 | 1 | 13 | 1 | 2 | 2 | 22 | 1 | 2 | 3 |
| 5 | 2 | 2 | 1 | 14 | 2 | 2 | 2 | 23 | 2 | 2 | 3 |
| 6 | 3 | 2 | 1 | 15 | 3 | 2 | 2 | 24 | 3 | 2 | 3 |
| 7 | 1 | 3 | 1 | 16 | 1 | 3 | 2 | 25 | 1 | 3 | 3 |
| 8 | 2 | 3 | 1 | 17 | 2 | 3 | 2 | 26 | 2 | 3 | 3 |
| 9 | 3 | 3 | 1 | 18 | 3 | 3 | 2 | 27 | 3 | 3 | 3 |

To access the indices for a single mode, the vector can be re-shaped as a 3-dimensional tensor with the first index running over a multi-index of all the preceeding modes, the middle index the indices of the mode of interest, and the final index the multi-index for all the following modes.

As an example, for a 4D system with 3 SPFs per mode, the A-vector can be re-shaped around the 3rd mode

$$A_J \longrightarrow A_{J_v j_3 J_n} \Rightarrow \mathrm{Avector}(J_v, j_3, J_n)$$

where in this case the final index runs over the indices of the fourth mode, $J_n = j_4$ and there are 9 indices for the first dimension as listed in Table 2

Table 2: The A-vector indices for the combined 2D first index of a 4D system with 3 SPFs per mode

| vector index $J$ | Mode indices $j_1$ | $j_2$ |
|---|---|---|
| 1 | 1 | 1 |
| 2 | 2 | 1 |
| 3 | 3 | 1 |
| 4 | 1 | 2 |
| 5 | 2 | 2 |
| 6 | 3 | 2 |
| 7 | 1 | 3 |
| 8 | 2 | 3 |
| 9 | 3 | 3 |

## 1.2 The SPFs

The single-particle functions are defined as a vector on the underlying DVR grid for each function. Thus they are stored as matrices

$$\varphi_i(q,t) \longrightarrow \varphi_i(q_\alpha, t) \Rightarrow \mathrm{SPF}(\alpha, i)$$

where the index $\alpha$ runs over the grid points and $i$ over the functions. For a multi-set wavefunction there are $n_s$ sets of functions. The program `rd`spfs writes the sets of functions as vectors.

In a Quantics calculation, if the grid is a DVR then integrals of potential functions are evaluated using a quadrature formalism (see Beck et al Phys. Rep. (2000) 324:1 for details)

$$\langle \varphi_i | h | \varphi_j \rangle = \sum_\alpha w_\alpha \varphi_i(q_\alpha) h(q_\alpha) \varphi_j(q_\alpha)$$

i.e. summing over the value of the SPFs and operator at the DVR grid points.

For ease of manipulation, the SPFs are stored multiplied by the (square-root) of the DVR weights

$$\mathrm{SPF}(\alpha, i) = \sqrt{w_\alpha} \varphi_i(q_\alpha)$$

The program `rd`spfs by default will write out these weighted values. Non-weighted values can be obtained with the option `-`nw.

If there is an electronic DOF, then in a multi-set formalism the SPFs for different states are not orthonormal. For a single-set wavefunction there will also be a set of SPFs for the electronic basis. These are vectors relating an SPF to an electronic state.

## 2 The G-MCTDH wavefunction

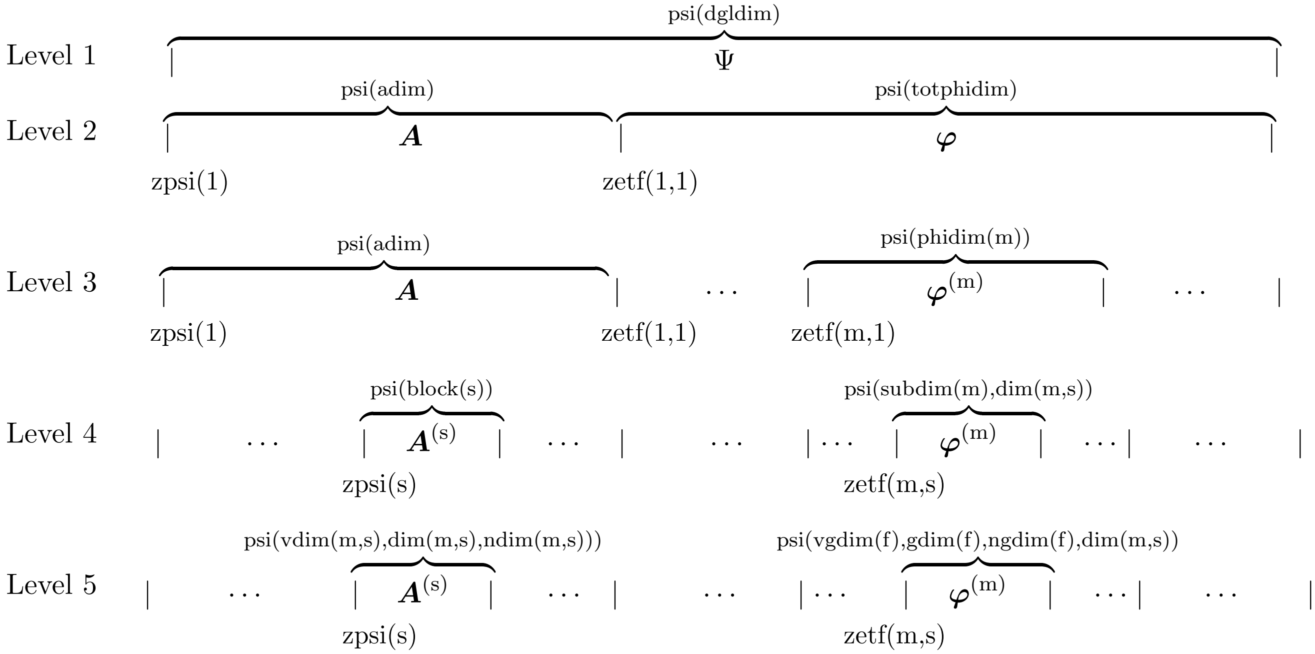
In G-MCTDH wavefunction some or all of the SPFs may be replaced by Gaussian basis frunctions (GBFs). I.e. in a multi-set function

$$\Psi(\boldsymbol{q},t) = \sum_{s=1}^{n_s} \sum_{j_1^s \dots j_f^s}^{N} A_{j_1^s \dots j_f^s}(t) \varphi_{j_1^s}^{(\kappa)}(q_1,t) \cdots \varphi_{j_n^s}^{(\kappa)}(q_n,t) g_{j_{n+1}^s}^{(\kappa)}(q_{n+1},t) \cdots g_{j_f^s}^{(\kappa)}(q_f,t)$$

The A-coefficients and SPFs are stored as in a standard MCTDH function. The A-coefficients vector, however, is no longer normalised. The GBFs have the form

$$g_i = \sum_{\alpha\beta} = \zeta_{i,\alpha\beta} x_\alpha x_\beta + \xi_{i,\alpha} x_\alpha + \eta_i$$

and the parameters $\zeta, \xi, \eta$ and written out by `r`dspfs.



- Level 1. The whole wavefunction is stored in the array "psi" which has a length "dgldim".

- Level 2. The A coefficient vector has length "adim" starting from the pointer "zpsi(1)". The SPFs are stored in memory of length "totphidim" starting at "zetf(1,1)"

- Level 3. The SPFs for mode $m$ are stored in memory of length "phidim(m)" starting at "zetf(m,1)"

- Level 4. The A coefficient vector for state $s$ has length "block(s)" starting from the pointer "zpsi(s)". The SPFs for mode $m$ and state $s$ are a matrix of dimensions "subdim(m) × dim(m,s)" starting at "zetf(m,s)"

- Level 5. Finally, the A coefficient vector can be reshaped to use the indices for the SPF of mode / state $m, s$ as a tensor with dimensions "vdim(m,s) × dim(m,s) × ndim(m,s). The SPF grids can likewise be broken down to index for the DOF $f$ by reshaping "subdim(m) × dim(m,s)" to "vgdim(f) × gdim(f) × ngdim(f) × dim(m,s)".

Figure 1: The pointer structure of the `psi` array