CDVR Algorithm

The CDVR algorithm (Manthe JCP 1996 **105**: 6989) is a time dependent DVR with a correction to treat separable components of the Hamiltonian exactly.

We have three bases:
The SPF basis $|\varphi^{(\kappa)}_{j_\kappa}\rangle$
The DVR basis on the points x, $|X^{(\kappa)}_{x_\kappa}\rangle$
The TDDVR basis on the points q, $|Q^{(\kappa)}_{q_\kappa}\rangle$
where the latter are the eigenvalues $q^{(\kappa)}$ and eigenvectors $U^{(\kappa)}_{qj} = \langle Q^{(\kappa)}_q|\varphi^{(\kappa)}_j\rangle$ of the position operator in the spf basis $\langle\varphi^{(\kappa)}_j|x|\varphi^{(\kappa)}_m\rangle$. The matrix $D^{(\kappa)}_{qj} = \langle X^{(\kappa)}_q|\varphi^{(\kappa)}_j\rangle$ is the definition of the SPF basis in the DVR basis.

To evaluate a matrix element in the TDDVR basis:
$\langle Q^{(1)}_{j_1}\cdots Q^{(f)}_{j_f}|V(x_1,\cdots,x_f)|Q^{(1)}_{m_1}\cdots Q^{(f)}_{m_f}\rangle = V(q^{(1)}_{j_1}\cdots q^{(f)}_{j_f})\delta_{j_1m_1}\cdots\delta_{j_fm_f} +$
$\sum_{\kappa=1}^f\langle Q^{(\kappa)}_{m_\kappa}|\Delta V(q^{(1)}_{j_1}\cdots q^{(\kappa-1)}_{j_\kappa-1},x_\kappa,q^{(\kappa+1)}_{j_\kappa+1}\cdots q^{(f)}_{j_f}|Q^{(\kappa)}_{m_\kappa}\rangle\delta_{j_1m_1}\cdots\delta_{j_{\kappa-1}m_{\kappa-1}}\delta_{j_{\kappa+1}m_{\kappa+1}}\cdots\delta_{j_fm_f}$
where the first term on the RHS is the approximation that the potential is diagonal on the TDDVR points, and the second term is the CDVR correction: $\langle Q^{(\kappa)}_{m_\kappa}|\Delta V(q^{(1)}_{j_1}\cdots q^{(\kappa-1)}_{j_\kappa-1},x_\kappa,q^{(\kappa+1)}_{j_\kappa+1}\cdots q^{(f)}_{j_f}\rangle =$

$\langle Q^{(\kappa)}_{m_\kappa}|V(q^{(1)}_{j_1}\cdots q^{(\kappa-1)}_{j_\kappa-1},x_\kappa,q^{(\kappa+1)}_{j_\kappa+1}\cdots q^{(f)}_{j_f}|Q^{(\kappa)}_{m_\kappa}\rangle - V(q^{(1)}_{j_1}\cdots q^{(f)}_{j_f})\delta_{j_\kappa m_\kappa}$

MCTDH Code

In **getcdvr**, the $q^{(\kappa)}$ and $U^{(\kappa)}_{qj}$ are calculated and stored for each mode.

In **matrizen4** the mean fields and time derivative of the A-coefficients is calculated , using the CDVR method.

1. Transform coefficients from spf to TDDVR basis:
   $B_{q_1\cdots q_f} = \sum_j U^{(1)}_{qj}\cdots U^{(f)}_{qj}A_{j_1\cdots j_f}$
2. Calculate mean fields and CDVR correction.
   do $\kappa = 1, f$
   (i) transform mode κ from TDDVR to DVR basis
   $B'_{q_1\cdots,x_\kappa,\cdots,q_f} = D^{(\kappa)}_{xj}U^{(\kappa)\dagger}_{qj}B_{q_1\cdots q_\kappa\cdots q_f}$
   (ii) operate on B
   $B^V_{q_1\cdots,x_\kappa,\cdots,q_f} = V(q_1\cdots,x_\kappa,\cdots,q_f)B'_{q_1\cdots,x_\kappa,\cdots,q_f}$
   (iii) form meanfield matrix
   $H(x,q) = \sum B^*_{q_1\cdots,q_\kappa,\cdots,q_f}B^V_{q_1\cdots,x_\kappa,\cdots,q_f}$
   $H(x,j) = U^{(\kappa)\dagger}_{qj}H(x,q)$
   (iv) Calculate CDVR correction
   $C_{q_1\cdots,q_\kappa,\cdots,q_f} = U^{(\kappa)}_{q,j}D^{(\kappa)}_{x,j}B^V_{q_1\cdots,x_\kappa,\cdots,q_f}$

   enddo
3. calculate
   $V_{q_1\cdots,q_\kappa,\cdots,q_f} = V(q^{(1)}_{j_1}\cdots q^{(f)}_{j_f})$
4. calculate
   $i\dot{A}'_{q_1\cdots,q_\kappa,\cdots,q_f} = C_{q_1\cdots,q_\kappa,\cdots,q_f} - (f-1)V_{q_1\cdots,q_\kappa,\cdots,q_f}$
5. transform A from TDDVR to SPF basis
   $iA_{j_1\cdots j_f} = \sum_j U^{(1)\dagger}_{qj}\cdots U^{(f)\dagger}_{qj}A'_{q_1\cdots q_f}$