Operator functions

The following tables describe the symbols and related operators that can be used to set up a Hamiltonian operator.

General Remarks

With the aid of the caret ˆ one may apply a power to operators. The power may be integer or real and may carry a sign. This, however, works only for potential like operators. Inspect the Tables below to learn, which operators can be exponentiated. Note, that symbols like `dq^2` or `j^2` are operator labels of their own right, they do not denote that the second power of the operators `dx` or `j` is taken literally. (Compare with Appendix B (Discrete Variable Representation) of the MCTDH review (Phys.Rep. 324 (2000) 1-105), to learn how `dq` and `dq^2` are defined).

One may multiply operators, e.g. a construct like `dq*cos*dq` is allowed. However, multiplication is allowed only among potential like operators and operators with a simple matrix representation. This excludes all `KLeg` and `PLeg` operators from multiplication. (See Table 2 and notes to this table). Moreover, `natpots` cannot be multiplied with other operators. (See Section **??**)

Table 1: Simple one-dimensional operators. The expression x is the coordinate, r can be replaced by any real number, positive or negative. If $r = 1$ it is not required, e.g. q and qˆ1 are synonemous. The expression n can be replaced by any non-negative integer.

Symbol	Operator	Notes
1	1	Unit operator
I	i*1	Imaginary unit times unit operator
qˆr	x^r	Multiply by rth power of x
qsˆr	$(1-x^2)^{r/2}$	Multiply by rth power of $\sqrt{1-x^2}$
sinˆr	$\sin^r(x)$	rth power of sine of coordinate
cosˆr	$\cos^r(x)$	rth power of cosine of coordinate
tanˆr	$\tan^r(x)$	rth power of tangent of coordinate
coshˆr	$\cosh^r(x)$	rth power of hyperbolic-cosine of x
sinhˆr	$\sinh^r(x)$	rth power of hyperbolic-sine of x
acosˆr	$\arccos^r(x)$	rth power of acosine of coordinate
asinˆr	$\arcsin^r(x)$	rth power of asine of coordinate
atanˆr	$\arctan^r(x)$	rth power of atangent of coordinate
expˆr	$\exp(x)^r$	exponential of coordinate
texpˆr	$\exp(\arccos(x))^r$	exponential arc-cosine of coordinate
gaussˆr	$\exp(-x^2)^r$	gaussian of coordinate
tgaussˆr	$\exp(-\arccos(x)^2)^r$	gaussian of arc-cosine of coordinate
ngaussˆr	$\exp(-x^2/2)^r/\sqrt{2\pi}$	normalized gaussian
legth:n	$P_n(\cos(x))$	nth order Legendre polynomial of cosine of x
asleg:l_m	$P_l^m(x)$	associated Legendre polynomial of x (see function `plgndr` in sorce/lib/utilities/legendre.f)
aslegth:l_m	$P_l^m(\cos(x))$	associated Legendre polynomial of cosine of x
c_p	$\sqrt{J(J+1)-K(K+1)}$	C^+_{JK} symbol appearing with the j_+ operator (see Table 2). J is fixed.
c_m	$\sqrt{J(J+1)-K(K-1)}$	C^-_{JK} symbol appearing with the j_- operator (see Table 2). J is fixed.
my1d		user supplied routine. See Note 8 of Table 3.

Table 2: Operator symbols which require no arguments. The expression n can be replaced by any positive integer. Finally, m is the mass of the relevant degree of freedom. In the MCTDH input, this mass is given by the reserved parameter `mass_`*modelabel*. If `mass_`*modelabel* is not explicitely set, it is 1 by default.

Symbol	Operator	Notes
dq	∂_x	first derivative. Cannot be used for rHO, Leg, KLeg, PLeg, Wigner or sphFBR.
dqˆ2	∂_x^2	second derivative. Cannot be used for Leg, KLeg, PLeg, Wigner or sphFBR.
p	$-i\partial_x$	momentum (deprecated, use dq) When using an FFT, the construct pˆn is possible for integer n.
KE	$-\frac{1}{2m}\partial_x^2$	Kinetic energy term. Cannot be used for modes with a Legendre DVR or sphFBR.
jˆ2	$-\sin^{-1}(\theta)\,\partial_\theta \sin(\theta)\,\partial_\theta - \sin^{-2}(\theta)\,\partial_\phi^2$	Angular momentum squared. In this form used for sphFBR and PLeg. For Leg and KLeg ∂_ϕ^2 is replaced by $-m^2$ (or $-K^2$).
j_p	$e^{i\phi}\,(\partial_\theta + i\cot(\theta)\,\partial_\phi)$	Angular momentum raising operator j_+. Only for KLeg and PLeg. For Wigner see below.
j_m	$e^{-i\phi}\,(-\partial_\theta + i\cot(\theta)\,\partial_\phi)$	Angular momentum lowering operator j_-. Only for KLeg and PLeg. For Wigner see below.
jpm	$C_{JK}^{+}\,j_+ + C_{JK}^{-}\,j_-$	Combined angular momentum operator. $C_{JK}^{\pm}$ are defined in Table 1. Only for KLeg and PLeg.
cjpm	$C_{JK}^{+}(j_{1,+} + j_{2,+}) + C_{JK}^{-}(j_{1,-} + j_{2,-})$	Combined operator for two angular momenta. Here $K = k_1 + k_2$, so this is different from jpm for the two individual angular momenta. Only for two successive KLegs, which furthermore have to be combined in one mode.
jz	$j_z = -i\partial_\phi$	Angular momentum operator. Only for sphFBR and KLeg. For PLeg use dq or p on the ϕ DOF.
jzˆ2	$j_z^2 = (-i\partial_\phi)^2$	second power of angular momentum operator j_z. Only for sphFBR and KLeg. For PLeg use dqˆ2 on the ϕ DOF.
jpˆ2	$(j_+)^2$	Square of angular momentum raising oper-

Table 2, continued.

Symbol	Operator	Notes
jmjp	$(j_-) * (j_+)$	Product of angular momentum lowering and raising operators. Only for KLeg and PLeg.
sJp	$\sin(\theta) * J_+$	J is total angular momentum. Only for KLeg and PLeg.
sJm	$\sin(\theta) * J_-$	J is total angular momentum. Only for KLeg and PLeg.
sJpk	$(\sin(\theta) * J_+ * k + k * sin(\theta) * J_+)/2$	Only for KLeg and PLeg.
sJmk	$(\sin(\theta) * J_- * k + k * sin(\theta) * J_-)/2$	Only for KLeg and PLeg.
Jp	J_+	multiplication with C^-_{JK} and shift $k \to k-1$
Jm	J_-	multiplication with C^+_{JK} and shift $k \to k+1$
Jx	J_x	$J_x = (J_+ + J_-)/2$
Jy	iJ_y	$iJ_y = (J_+ - J_-)/2$
dth1	$\partial_\theta \, \sin\theta$	"first derivative", only for Leg- KLeg- and PLeg-DVR (no symmetry).
dth2	$\frac{1}{2}(\cos\theta \, \partial_\theta \, \sin\theta + \partial_\theta \, \sin\theta \, \cos\theta)$	"first derivative", only for Leg- KLeg- and PLeg-DVR (symmetry).
qdq	$\frac{1}{2}(x \, \partial_x + \partial_x \, x)$	for rHO-DVR this replaces the "first derivative".
sdq	$\frac{1}{2}(\sin(x) \, \partial_x + \partial_x \, \sin(x))$	for cos-DVR this replaces the "first derivative".
sdq2	$\frac{1}{2}(\sin^2(x) \, \partial_x + \partial_x \, \sin^2(x))$	
cdq	$\frac{1}{2}(\cos(x) \, \partial_x + \partial_x \, \cos(x))$	
cdq2	$\frac{1}{2}(\cos^2(x) \, \partial_x + \partial_x \, \cos^2(x))$	
csdq	$\frac{1}{2}(\sin(x)\cos(x) \, \partial_x + \partial_x \, \sin(x)\cos(x))$	
udq	$\frac{1}{2}(\sqrt{1-x^2} \, \partial_x + \partial_x \, \sqrt{1-x^2})$	
uqdq	$\frac{1}{2}(\sqrt{1-x^2} \, x \, \partial_x + \partial_x \, \sqrt{1-x^2} \, x)$	
udq2	$\frac{1}{2}((1-x^2) \, \partial_x + \partial_x \, (1 -4x^2))$	
p%<integer>		p%k is a projector which projects onto the momentum state which is

Table 2, continued.

Symbol	Operator	Notes
j^2	$-\partial_\beta^2 - \cot(\beta)\,\partial_\beta - \sin^{-2}(\beta)\,[\partial_\alpha^2 + \partial_\gamma^2 - 2\cos(\beta)\,\partial_\alpha\,\partial_\gamma]$	Wigner-DVR angular momentum squared operator, with matrix elements: $j^2\,\lvert J,K,M\rangle = J(J+1)\,\lvert J,K,M\rangle$.
j_p	$(j_+)_{\mathrm{BF}} = e^{-i\gamma}\left(\frac{i}{\sin(\beta)}\partial_\alpha + \partial_\beta - i\cot(\beta)\,\partial_\gamma\right)$	Wigner-DVR body-fixed angular momentum lowering operator, which operates as: $(j_+)_{\mathrm{BF}}\,\lvert J,K,M\rangle = \sqrt{J(J+1) - K(K-1)}\,\lvert J,K-1,M\rangle$.
j_m	$(j_-)_{\mathrm{BF}} = e^{i\gamma}\left(\frac{i}{\sin(\beta)}\partial_\alpha - \partial_\beta - i\cot(\beta)\,\partial_\gamma\right)$	Wigner-DVR body-fixed angular momentum raising operator, which operates as: $(j_-)_{\mathrm{BF}}\,\lvert J,K,M\rangle = \sqrt{J(J+1) - K(K+1)}\,\lvert J,K+1,M\rangle$.
j_ps	$(j_+)_{\mathrm{SF}} = e^{i\alpha}\left(i\cot(\beta)\partial_\alpha + \partial_\beta - \frac{i}{\sin(\beta)}\partial_\gamma\right)$	Wigner-DVR space-fixed angular momentum raising operator, which operates as: $(j_+)_{\mathrm{SF}}\,\lvert J,K,M\rangle = \sqrt{J(J+1) - M(M+1)}\,\lvert J,K,M+1\rangle$.
j_ms	$(j_-)_{\mathrm{SF}} = e^{-i\alpha}\left(i\cot(\beta)\partial_\alpha - \partial_\beta - \frac{i}{\sin(\beta)}\partial_\gamma\right)$	Wigner-DVR space-fixed angular momentum lowering operator, which operates as: $(j_-)_{\mathrm{SF}}\,\lvert J,K,M\rangle = \sqrt{J(J+1) - M(M-1)}\,\lvert J,K,M-1\rangle$.
jpm	$C^+_{JK}\,(j_-)_{\mathrm{BF}} + C^-_{JK}\,(j_+)_{\mathrm{BF}}$	Wigner-DVR body-fixed combined angular momentum operator. $C^\pm_{JK}$ are defined in Table 1.
jpms	$C^+_{JM}\,(j_+)_{\mathrm{SF}} + C^-_{JM}\,(j_-)_{\mathrm{SF}}$	Wigner-DVR space-fixed combined angular momentum operator. $C^\pm_{JM}$ are defined in Table 1, but here M replaces K.
jp^2	$(j_+)^2_{\mathrm{BF}}$	Wigner-DVR squared body-fixed angular momentum raising operator.
jp^2s	$(j_+)^2_{\mathrm{SF}}$	Wigner-DVR squared space-fixed angular momentum raising operator.
jm^2	$(j_-)^2_{\mathrm{BF}}$	Wigner-DVR squared body-fixed angular momentum lowering operator.
jm^2s	$(j_-)^2_{\mathrm{SF}}$	Wigner-DVR squared space-fixed angular momentum lowering operator.

(continued)

Table 2, continued.

Symbol	Operator	Notes
jpjm	$(j_+)_{\rm BF} * (j_-)_{\rm BF}$	Wigner-DVR product of body-fixed angular momentum raising and lowering operators.
jpjms	$(j_+)_{\rm SF} * (j_-)_{\rm SF}$	Wigner-DVR product of space-fixed angular momentum raising and lowering operators.
jmjp	$(j_-)_{\rm BF} * (j_+)_{\rm BF}$	Wigner-DVR product of body-fixed angular momentum lowering and raising operators.
jmjps	$(j_-)_{\rm SF} * (j_+)_{\rm SF}$	Wigner-DVR product of space-fixed angular momentum lowering and raising operators.
jpjz	$(j_+)_{\rm BF} * (j_z)_{\rm BF}$	Wigner-DVR product of body-fixed angular momentum operators, which operates as: $(j_+)_{\rm BF}(j_z)_{\rm BF}\,\|J,K,M\rangle = K\sqrt{J(J+1)-K(K-1)}\,\|J,K-1,M\rangle$.
jpjzs	$(j_+)_{\rm SF} * (j_z)_{\rm SF}$	Wigner-DVR product of space-fixed angular momentum operators, which operates as: $(j_+)_{\rm SF}(j_z)_{\rm SF}\,\|J,K,M\rangle = M\sqrt{J(J+1)-M(M+1)}\,\|J,K,M+1\rangle$
jzjp	$(j_z)_{\rm BF} * (j_+)_{\rm BF}$	Wigner-DVR product of body-fixed angular momentum operators, which operates as: $(j_z)_{\rm BF}(j_+)_{\rm BF}\,\|J,K,M\rangle = (K-1)\sqrt{J(J+1)-K(K-1)}\,\|J,K-1,M\rangle$.
jzjps	$(j_z)_{\rm SF} * (j_+)_{\rm SF}$	Wigner-DVR product of space-fixed angular momentum operators, which operates as: $(j_z)_{\rm SF}(j_+)_{\rm SF}\,\|J,K,M\rangle = (M+1)\sqrt{J(J+1)-M(M+1)}\,\|J,K,M+1\rangle$
jmjz	$(j_-)_{\rm BF} * (j_z)_{\rm BF}$	Wigner-DVR product of body-fixed angular momentum operators, which operates as: $(j_-)_{\rm BF}(j_z)_{\rm BF}\,\|J,K,M\rangle = K\sqrt{J(J+1)-K(K+1)}\,\|J,K+1,M\rangle$.
jmjzs	$(j_-)_{\rm SF} * (j_z)_{\rm SF}$	Wigner-DVR product of

Notes to Table 2

The volume-element assumed for Leg/KLeg/PLeg/Wigner is $\sin\theta\, d\theta$, whereas all other DVRs in MCTDH assume the simple volume-element dq. Because of the non-trivial volume-element, ∂_θ is not an anti-hermitian operator, only $\partial_\theta \sin\theta$ (i.e. dth1) is. Note that $\sin\theta\, \partial_\theta = \partial_\theta \sin\theta - \cos\theta = \text{dth1} - \cos\theta$.

The operators j_p, j_m, jpm, jp^2 and jm^2 are (KLeg or PLeg) 2D mode-operators, i.e. they operate on the combined mode (θ,k) or (θ,ϕ) for KLeg or PLeg, respectively. Note that j^2 becomes a 2D mode-operator, when operating on a KLeg or PLeg mode. Similarly, the operators sJp, sJm, sJpk, and sJmk are also 2D KLeg/PLeg operators, where J denotes the total angular momentum. The 2D mode operator j_p performs a multiplicative and shift operation on k, but additionally performs a derivative and k-dependent multiplicative operation on the θ-dof of the KLeg mode. Similar operations are done by the j_m, sJp, sJm, sJpk, and sJmk operators.

The operators jz, jz^2, Jp, Jm, Jx, Jz are 1D operators and operate on the k-dof of the KLeg mode only. Hence they must appear in the k-column whereas the 2D KLeg-operators must appear under the θ column. (A more vivid way of writing the operator file is to let the 2D operator appear under both columns by using the `|&` construct, see Section **??**. However, in contrast to potential functions one must not reorder the DOFs of KLeg/PLeg/Wigner operators. For example `|2&3` is fine, but `|3&2` is not.)

When applied to Wigner functions, the operators j^2, j_p, j_m, jpm, jp^2, jm^2, jpjm, jmjp, jpjz, jzjp, jmjz, and jzjm are 3D mode operators and are represented as 4D tensors in MCTDH, so care must be taken when multiplying these operators with other operators. The Wigner operators j_p, j_m, jpm, jp^2, jm^2, jpjm, jmjp, jpjz, jzjp, jmjz, and jzjm operate in the BODY-fixed axis system; that is, these operators perform multiplicative operations and shifts depending on the k (second) degree of freedom in the combined 3D mode. The corresponding SPACE-fixed operators, which perform multiplications and shifts depending on the m (third) DOF, are denoted j_ps, j_ms, jpms, jp^2s, jm^2s, jpjms, jmjps, jpjzs, jzjps, jmjzs, and jzjms. Note that j_+ and j_- are defined as $j_+ = j_x + ij_y$ and $j_- = j_x - ij_y$ for both the SF- and BF-system. Due to the anomalous commutation relation for the BF operators, j_p = $(j_+)_{BF}$ *decreases* k by one, whereas j_ps = $(j_+)_{SF}$ increases m by one.

The operator cjpm is a 4D mode-operator (two successive KLegs). It only works if the two KLegs are combined into one mode, and for this case it replaces the use of natural potentials of the cpp/cmm surfaces (see Table 5).

Note that the operators j_p, j_m, jpm, cjpm, jp^2, jm^2, sJp, sJm, sJpk and sJmk — as well as j^2 if the latter operates on a KLeg/PLeg combined mode — are 3D tensors in MCTDH and not matrices. Hence care must be taken when multiplying these operators with other operators. To give an example

```
HAMILTONIAN-SECTION
```

Table 2, continued.

Symbol	Operator	Notes
jzjm	$(j_z)_{\mathrm{BF}} * (j_-)_{\mathrm{BF}}$	Wigner-DVR product of body-fixed angular momentum operators, which operates as: $(j_z)_{\mathrm{BF}}(j_-)_{\mathrm{BF}}\,\|J,K,M\rangle = (K+1)\sqrt{J(J+1)-K(K+1)}\,\|J,K+1,M\rangle$.
jzjms	$(j_z)_{\mathrm{SF}} * (j_-)_{\mathrm{SF}}$	Wigner-DVR product of space-fixed angular momentum operators, which operates as: $(j_z)_{\mathrm{SF}}(j_-)_{\mathrm{SF}}\,\|J,K,M\rangle = (M-1)\sqrt{J(J+1)-M(M-1)}\,\|J,K,M-1\rangle$
AA	a	Annihilation operator in second quantization. Upper side-diagonal is $(\sqrt{1}, \sqrt{2}, \cdots, \sqrt{\mathrm{gdim}-1})$, all other matrix elements are zero.
AD	$a^\dagger$	Creation operator in second quantization. Lover side-diagonal is $(\sqrt{1}, \sqrt{2}, \cdots, \sqrt{\mathrm{gdim}-1})$, all other matrix elements are zero.
AP	$a + a^\dagger$	Operator in second quantization.
AM	$a - a^\dagger$	Operator in second quantization.
NN	$a^\dagger a$	Number operator in second quantization.

```
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  modes   | ... |  theta  |  k
-----------------------------------
 ...      | ... | cos*j_p | c_p
 ...      | ... | j_p*cos | c_p
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end-hamiltonian-section
```

is a valid construct. Note that the 2D operator j_p may be multiplied from right or left with and operator operating on θ only. However, it may be multiplied only from right with a local k-dependent function (here c_p).

The operators dth1, dth2, qdq, and sdq replace the first derivative operator for the Leg (and KLeg/PLeg), rHO, cos (and sin when the keyword sdq is given) DVR, repectively. In these cases the operator dq cannot be used.

The operators AA, AD, AP, AM, and NN are fro treating vibrations or bosonic systems in second quantization. For the respective DOFs it is convenient to use a sin-DVR which starts at zero and has a mesh width of 1. E.g.: `q1 sin 12 0.0 11.0`

Table 3: One-dimensional operators which require arguments. The expression x stands for the coordinate, p can be replaced by any parameter from the PARAMETER-SECTION, or any real number. The exponent r can be any real number. If $r = 1$ it is not required, e.g. $q[p]$ and $q[p]$ˆ1 are synonemous.

Symbol	Operator
q[p]ˆr	$(x-p)^r$
qs[p]ˆr	$(\sqrt{p-x^2})^r$
sin[p1,p2]ˆr	$\sin^r(p1(x-p2))$
cos[p1,p2]ˆr	$\cos^r(p1(x-p2))$
tan[p1,p2]ˆr	$\tan^r(p1(x-p2))$
exp[p1,p2]ˆr	$\exp^r(p1(x-p2))$
Exp[p1,p2]ˆr	$\exp^r(i*p1(x-p2))$
texp[p1,p2]ˆr	$\exp^r(p1(\arccos(x)-p2))$
sinh[p1,p2]ˆr	$\sinh^r(p1(x-p2))$
cosh[p1,p2]ˆr	$\cosh^r(p1(x-p2))$
tanh[p1,p2]ˆr	$\tanh^r(p1(x-p2))$
cos1[p1,p2]ˆr	$(\cos(p1*x)-\cos(p1*p2))^r$
exp1[p1,p2]ˆr	$(1-\exp(p1(x-p2)))^r$
expcos[p1,p2]ˆr	$(\exp(p1\cos(x))-\exp(p1\cos(p2)))^r$
expcos1[p1,p2]ˆr	$\exp(p1(\cos(x)-p2))^r$
qtanh[p1,p2,p3]ˆr	$\tanh^r(p2(\arccos(x)-p1)^{p3})$
motanh[p1,p2,p3,p4]ˆr	$\tanh^r(p3[1-\exp(-p1(x-p2))]^{p4})$
asin[p1,p2,p3]ˆr	$(\arcsin(p1*x-p2)-p3)^r$
acos[p1,p2,p3]ˆr	$(\arccos(p1*x-p2)-p3)^r$
atan[p1,p2,p3]ˆr	$(\arctan(p1*x-p2)-p3)^r$
coschirp[p1,p2,p3]ˆr	$\cos^r(x[p2+(p1-p2)\exp(-(x/p3)^2)])$
tgauss[p1,p2]ˆr	$\exp(-p1(\arccos(x)-p2)^2)^r$
gauss[p1,p2]ˆr	$\exp(-p1(x-p2)^2)^r$
ngauss[σ, x_0]ˆr	$(2\pi\sigma^2)^{-1/2}\exp(-(x-x_0)^2/(2\sigma^2))^r$
morse[p1,p2,p3,p4,p5]	Morse function. See Note 1.
morse1[p1,p2,p3,p4]	Morse function. See Note 1.
CAP[p1,p2,p3,p4]	$-iW$. See Note 2.
ACAP[p1,p2,p3,p4,p5]	$-iW$. See Note 3.
switch1[p1,p2]	$0.5*[1-\tanh(p1(x-p2))]$
switch2[p1,p2]	$0.5*[1+\tanh(p1(x-p2))]$
step[p]	$\Theta(x-p)$ Step function. See Note 4.
rstep[p]	$\Theta(p-x)$ Reverse step function. See Note 4.
charfun[p1,p2]	characteristic function: if $x \in [p1,p2]$ then charfun=1 else it is zero.
regcoul[p1,p2]	regularized coulomb function: $1/\sqrt{(x-p1)^2+p2}$.
low[m, ω, s]	lowering operator. See Note 5.
rai[m, ω, s]	raising operator. See Note 5.
num[m, ω, s]	number operator. See Note 5.

(continued)

Table 3, continued.

Symbol	Operator
ramorse[$m, \omega, \Lambda, \alpha, z_0$]	raising operator for Morse potential. See Note 6.
lwmorse[$m, \omega, \Lambda, \alpha, z_0$]	lowering operator for Morse potential. See Note 6.
cspot[$J, K, csmax, m$]	centrifugal potential. See Note 7.
external1d{*file*}	external 1D function read from file *file*. See Note 8.
read1d{*file F*}	external 1D function read from file *file* of format *F*. See Note 9.
my1d[p1,p2,p3,p4,p5]	user supplied routine. See Note 10.
flux[$x_c, power$]	Flux operator for Cartesian kinetic energy. x_c = location of dividing surface, *power* = exponent of smoothing function. See Note 11.
pgauss[σ, x_0]	Projector $\|G >< G\|$, where G denotes a L^2 normalized Gauss $G = (2\pi\sigma^2)^{-1/4}\, exp[-(x-x_0)^2/(4\sigma^2)]$
shift[Ω]	simple shift on the grid by Ω, $\tilde{\psi}(x_i) = \psi(x_{i-\Omega})$ $\tilde{\psi}(x_i) = 0$ if $i - \Omega < 1$ or $i - \Omega > N$ For a periodic shift on a periodic grid (exp-DVR of FFT) use shift[Ω] and shift[$\Omega - N$] (with $\Omega > 0$).
vecpot[A_0, ω, N_c]	$A(x) = A_0 \cos(\omega x - N_c\pi)\sin^2(\frac{\omega x}{2N_c})$. Vector potential for linearly polarized pulse. A_0, ω and N_c are the amplitude, frequency and number of cycles of the pulse, respectively.
Peierls[l, ω, N_c]	Peierls' phase: $\exp(il\cos(\omega x - N_c\pi)\sin^2(\frac{\omega x}{2N_c}))$.

Table 4: One-dimensional potential energy curves.

Symbol	Potential Curve
v:NO	NO potential curve
v:H2	H_2 potential (link lsth)
vbmkp:H2	H_2 potential (link h4bmkp)
v:HO	OH potential, morse function from h2o.f
v:OH	OH potential (link hoosrf)
v:CH	CH potential (link c2h)
v:C2	C_2 potential (link c2hasec)
v:OF	OF potential curve
vrho:H3	H+H_2 potential in hypersphaerical coordinates, theta=π (link lsth)
vthe:H3	H+H_2 potential in hypersphaerical coordinates, rho=2.484773 (link lsth)
vdj:000	expansion coeffiecent V_{000} for DJ H_4 surface (link h4dj)
vdj:022	expansion coeffiecent V_{022} for DJ H_4 surface (link h4dj)
vdj:224	expansion coeffiecent V_{224} for DJ H_4 surface (link h4dj)

Table 5: Two-dimensional operators (used for molecule-surface scattering).

Symbol	Operator
coshcosth[p]	$\cosh(p * \cos(\theta))$
sinhcosth[p]	$\sinh(p * \cos(\theta))$
cossinthcosphi[p]	$\cos(p * \sin(\theta) * \cos(\phi))$
cossinthsinphi[p]	$\cos(p * \sin(\theta) * \sin(\phi))$
sinsinthcosphi[p]	$\sin(p * \sin(\theta) * \cos(\phi))$
sinsinthsinphi[p]	$\sin(p * \sin(\theta) * \sin(\phi))$
reY[l,m]	$\mathrm{Re}(Y_l^m(\theta, \phi))$
imY[l,m]	$\mathrm{Im}(Y_l^m(\theta, \phi))$

Table 6: Multi-dimensional C_+, C_- symbols defined on truncated k_1,k_2,...,k_d grid.

See also "Hamiltonian Documentation"/"Available Surfaces"

Symbol	Operator
cpp{jtot=J,dim=d}	$\sqrt{J(J+1) - (\sum_{j=1}^{d} k_j)(\sum_{j=1}^{d} k_j + 1)}$
cmm{jtot=J,dim=d}	$\sqrt{J(J+1) - (\sum_{j=1}^{d} k_j)(\sum_{j=1}^{d} k_j - 1)}$

Table 7: Some general multi-dimensional operators. Here parameters are to be given in curly brackets.
E.g: coulomb1d{a=1.3 b=2.0 c=0.0 d=1.5}. See also "Hamiltonian Documentation"/"Available Surfaces"

Symbol	Operator
readsrf{*file* F}	Potential values on grid points are read from file *file* of format F. (F=`ascii` or `binary`. See HTML Docu. For 1D-potential use read1d).

gauss1d{width=w S}	$\exp(-0.5((x_1 - x_2)/w)^2)/(\sqrt{2\pi}\, w)$
	If the optional string S is set to `periodic`,
	then a 2 π periodic grid is assumed.
	In this case the DVR lines should read e. g.:
	`x1 FFT 128 2pi`
	`x2 FFT 128 2pi`

gauss2d{width=w}	$\exp(-0.5([(x_1 - x_2)/w]^2 + [(y_1 - y_2)/w]^2))/(2\pi\, w^2)$
coulomb1d{$\cdots$}	$1/\sqrt{(a\, x_1 - b\, x_2 + c)^2 + d}$

Notes to Table 3

All input variables $[\cdots]$ are numbers, parameters or arithmetic expressions containing numbers and parameters. (See Hamiltonian-Documentation/Parameter-Section for details). The use of units is not allowed here. Note that these symbolic expressions with parameters must not appear in a HAMILTONIAN-SECTION. They rather have to be linked to simple symbols (without parameters) in a LABELS-SECTION. (Compare with Example 6.4).

1. A morse curve can be given by $D\,(\exp(-\alpha(x - x_0)) - 1)^2 + E_0$, where D is the dissociation energy (depth parameter), α defines the curvature, x_0 the equilibrium position, and E_0 is an energy shift parameter. If one uses the symbol morse1 these are precisely the input parameters, i.e. $[D, \alpha, x_0, E_0]$. For the symbol morse the input parameters are $[D, \omega, x_0, ex_0, m]$, where m is the mass, ω is the frequency of the related harmonic oscillator, and ex_0 is the position at which the potential is zero. Note that ω and α are related by $\alpha^2 = m\omega^2/2D$, while ex_0 and E_0 are related by $E_0 = -D(exp(-\alpha(ex_0 - x_0)) - 1)^2$.

2. A CAP (Complex Absorbing Potential) is an imaginary, negative potential, used to absorb a wavepacket as it approaches the end of the grid. It is defined as $-iW$, where $W = \eta\,\Theta(k(x - x_0))\,(k(x - x_0))^n$ and where Θ denotes the Heaviside's step function. The input parameters are $[x_0, \eta, n, k]$, where

Table 8: One-dimensional operators for treating symmetric double-well potentials by mapping each side on an artificial (single-set) electronic state. Note, the grid must be a sin-DVR, which, when doubled, lies symmetrically to zero but does not contain zero. The differential operators which are truncated are firstly defined on this doubled grid, but then projected to the working grid.

Symbol	Operator	Notes
Rf	$\mathrm{Rf}\,\varphi(x_i) = \varphi(x_{N+1-i})$	Reflection operator. (Must not be multiplied with other operators).
Rfm	$\mathrm{Rfm}\,\varphi(x_i) = -\varphi(x_{N+1-i})$	Reflection operator. (Must not be multiplied with other operators).
hKEh	step*KE*step	Truncated kinetic energy
hFRh	step*KE*Rf*step	Truncated kinetic energy times reflection
hdqh	step*dq*step	Truncated first derivative
hdqRh	step*dq*Rf*step	Truncated first derivative times reflection
dqR	dq*R	First derivative times reflection
dq2R	dq^2*R	Second derivative times reflection

k is used to choose to which end of the grid the CAP is placed: $k = -1$ puts the CAP at the left, and $k = 1$ at the right of the grid. $k = 1$ is default and may be left out.

3. ACAP symbolises an automatic CAP. The ACAP is useful, when one wants to place the initial wavepacket at a position, where it overlaps with the CAP. The ACAP remains disabled as long as the wavepacket overlaps with the CAP. The ACAP is enabled only when the wavepacket starts to re-enter the region where the CAP is defined. There is a fifth parameter: *timecap*. If this optional parameter is set, the ACAP will remain disabled at least as long as *time* $<$ *timecap*, where *time* is the propagation time in fs. The parameter *timecap* is useful, because the automatic enabling of the CAP may sometimes happen too early. The time, at which the ACAP is switched on, is protocoled in the `log` file. Use this information to set the option `-lo` in **flux84** appropriately. When **flux84** is run, it must not evaluate matrix elements of the CAP for times, at which the CAP is switched off.

4. The symbols step and rstep symbolise a Heaviside's step function and the reverse of it. I. e. step[p] $= \Theta(x-p)$ and rstep[p] $= 1-\Theta(x-p) = \Theta(p-x)$.

5. The lowering operator corresponding to a harmonic oscillator is given by

$$b = \frac{i}{\sqrt{2m\omega}}p + \sqrt{\frac{m\omega}{2}}(q - q_0)\,,$$

where p denotes the momentum operator, q denotes the position operator, m is the mass, ω is the frequency, and q_0 is the equilibrium position. The input parameters are $[m, \omega, s]$, which means the mass m, the frequency ω, and the shift

$$s = -\sqrt{\frac{m\omega}{2}} q_0 \,.$$

(Note the minus sign). The corresponding raising operator is given by $b^\dagger$, and the number operator by $\hat{n} = b^\dagger b$. The parameters have the same meaning as for lowering operators. NB. The lowering, raising and number operator require the use of a simple DVR with an ordinary first derivative, e.g. sin, HO, or exp but not FFT, rHO, Leg, KLeg, PLeg or sphFBR.

6. The (approximate) raising/lowering operators (R/L) for a Morse Hamiltonian

$$H = p^2/(2m) + D\left(e^{-2\alpha(x-x_0)} - 2e^{-\alpha(x-x_0)}\right)$$

are defined as

$$L = \sqrt{\frac{\hbar}{2m\omega}} \left[\left(\Lambda - \frac{1}{2}\right)\alpha - \Lambda\alpha e^{-\alpha(x-x_0)} + \frac{i}{\hbar}p\right]$$

and

$$R = L^\dagger$$

with $\omega = \alpha\sqrt{2D/m}$ and $\Lambda = \sqrt{2Dm}/\hbar\alpha$

7. The centrifugal potential given by:

$$V_{cent}(x) = min\left(\frac{J(J+1) - 2K^2}{2mx^2}\ ,\ csmax\right) \,.$$

8. An arbitrary (real) 1D–function may be defined through a set of points. The points are read from file *file* and are then interpolated to define a general 1D–function. The data is in free format with one (x,y) data pair per line. Blank lines and lines which start with a # are ignored. Currently, the x-data (called *time* in the code) must increase linearly, i.e must be equally spaced.

   An arbitrary number of these, with different data files, may be used in one operator. However, when using multiple instances of the same external1d function, do this by defining a label and referring to it in the operator rather than declaring external1d{*file*} with the same file *file* repeatedly, as this wastes buffer memory due to duplication.

9. An arbitrary (real) 1D–function may be defined through a set of points. The points must coincide with the grid points. The potential values on the

grip points are read from file *file*, one value per line. The file may be in ascii or binary format. (binary is default). Give `ascii` or `binary` as second argument after *file*. (For multi-dimensional surfaces use *readsrf*).

10. A (real) 1D–function may be defined through a user written subroutine. Edit the subroutine **my1d** on `$MCTDH_DIR/source/opfuncs/func1d.F` .

11. The flux operator $[\Theta, T]$ is set up in a sine or exponential basis and then transformed to DVR representation. This operator might be used with *eigenf* to produce flux-eigenstates as initial wavefunctions. To regularize the flux operator and to make its eigenfunctions more localized, it is multiplied from right and left with $[\cos(\pi p/2p_{max})\cosh(\pi p/2p_{max})]^{power}$. The exponent *power* may be zero or any positive real number. *power* = 1 is recommended.

Special operators

There is a number of operators especially defined for the methyl-iodine (CH3I) system. Their labels all start with MI: . See opfuncs/ch3i.f and opfuncs/ch3igrd.f for further information.

Non-adiabatic operators

If the system contains more than one electronic state, the Hamiltonian can be written in matrix form, i.e.

$$\hat{H} = \begin{pmatrix} H_{11} & H_{12} & \dots \\ H_{21} & H_{22} & \dots \\ \vdots & \vdots & \ddots \end{pmatrix} \tag{1}$$

To input such a form, the symbols in Table 9 can be used. Thus the operator

$$h_1 \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} + h_2 \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} + h_3 \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} \tag{2}$$

can be represented symbolically as

```
modes  | X   | el
1.0    | h_1 | 1
1.0    | h_2 | S1&2
1.0    | h_3 | Z1&2
```

See also Sec. **??** for more examples.

Table 9: Matrix operator symbols, used for an electronic degree of freedom.

Symbol	Operator
Sf&i	Symmetric matrix element
Zf&i	Unsymmetric matrix element
1	Unit matrix