In[240]:=
```
ClearAll["Global`*"]
```

In[241]:=
```
expand = NonCommutativeMultiply[ x___, Plus[y_, z_, w_], v___] →
   Plus[NonCommutativeMultiply[ x, y, v] +
     NonCommutativeMultiply[x, z, v] + NonCommutativeMultiply[x, w, v]];
(* to use the expand substitution rule repeatly: //.expand //ExpandAll *)
```

test the substitititution rule "expand"

In[242]:=
```
y ** (a + b + c ) ** x /. expand
```

Out[242]=
```
y ** a ** x + y ** b ** x + y ** c ** x
```

In[243]:=
```
y ** (a + b + w) /. expand
```

Out[243]=
```
y ** a + y ** b + y ** w
```

In[244]:=
```
(a + b + w) ** y /. expand
```

Out[244]=
```
a ** y + b ** y + w ** y
```

In[245]:=
```
(a + b + w) ** (m + n + k) //. expand
```

Out[245]=
```
a ** k + a ** m + a ** n + b ** k + b ** m + b ** n + w ** k + w ** m + w ** n
```

In[246]:=
```
2 ** (i + j + k) ** (u + v + w) ** (x + y + z) ** 9 //. expand
```

Out[246]=
```
2 ** i ** u ** x ** 9 + 2 ** i ** u ** y ** 9 + 2 ** i ** u ** z ** 9 +
 2 ** i ** v ** x ** 9 + 2 ** i ** v ** y ** 9 + 2 ** i ** v ** z ** 9 + 2 ** i ** w ** x ** 9 +
 2 ** i ** w ** y ** 9 + 2 ** i ** w ** z ** 9 + 2 ** j ** u ** x ** 9 + 2 ** j ** u ** y ** 9 +
 2 ** j ** u ** z ** 9 + 2 ** j ** v ** x ** 9 + 2 ** j ** v ** y ** 9 + 2 ** j ** v ** z ** 9 +
 2 ** j ** w ** x ** 9 + 2 ** j ** w ** y ** 9 + 2 ** j ** w ** z ** 9 + 2 ** k ** u ** x ** 9 +
 2 ** k ** u ** y ** 9 + 2 ** k ** u ** z ** 9 + 2 ** k ** v ** x ** 9 + 2 ** k ** v ** y ** 9 +
 2 ** k ** v ** z ** 9 + 2 ** k ** w ** x ** 9 + 2 ** k ** w ** y ** 9 + 2 ** k ** w ** z ** 9
```

get rid of ** in the places where they are not supposed to appear, ** are only supposed to appear on left and right side of P and $P^{\dagger}$.

In[247]:=
```
(*P and Pdag 's first element are P and SuperDagger[P] respectively*)
(* test if x is a single one and is an Integer or δ *)
ourtest[x_] :=
 If[ ( (Length[x] == 1) && (x[[1]] =!= P) && (x[[1]] =!= P†) ) || IntegerQ[x] || (x[[1]] == δ),
  True, False] (* when you use && and ||, remember to add brackets!!*)

(*move integer and δ to the front or the back*)
clean = NonCommutativeMultiply[x___, u_ /; ourtest[u], y___] :→
  Times[NonCommutativeMultiply[x, y], u]

clean2 =
  {
   (* one non-operator is in the middle of operators *)
   NonCommutativeMultiply[x__, u_ /; ourtest[u], y__] :→
    Times[NonCommutativeMultiply[x, y], u],
   (* one non-operator is at the end , and the number of operators is more than 2*)
   NonCommutativeMultiply[x__, y_, u_ /; ourtest[u]] :→
    Times[NonCommutativeMultiply[x, y], u],
   (* one non-operator is at the beginning ,
   and the number of operators is more than 2*)
   NonCommutativeMultiply[u_ /; ourtest[u], x_, y__] :→
    Times[NonCommutativeMultiply[x, y], u],
   (* one non-operator and one operator *)
   NonCommutativeMultiply[u_ /; ourtest[u], x_] :→ Times[x, u]
  };
```

Out[248]=
```
x___ ** (u_ /; ourtest[u]) ** y___ :→ x ** y u
```

In[250]:=
```
NonCommutativeMultiply[2, P] /. clean
```

Out[250]=
```
2 NonCommutativeMultiply[P]
```

test the substitution rule "clean"

In[251]:= $(P^{\dagger})_{j,m} ** P_{i,n} ** P_{j,m} ** (P^{\dagger})_{i,n1}$ //. clean

Out[251]= $(P^{\dagger})_{j,m} ** P_{i,n} ** P_{j,m} ** (P^{\dagger})_{i,n1}$

In[252]:= $(P^{\dagger})_{j,m} ** P_{i,n} ** P_{j,m} ** (P^{\dagger})_{i,n1} ** (-2)$ //. clean

Out[252]= $-2\ (P^{\dagger})_{j,m} ** P_{i,n} ** P_{j,m} ** (P^{\dagger})_{i,n1}$

In[253]:= $(P^{\dagger})_{j,m} ** P_{i,n} ** P_{j,m} ** (-2) ** (P^{\dagger})_{i,n1}$ //. clean

Out[253]= $-2\ (P^{\dagger})_{j,m} ** P_{i,n} ** P_{j,m} ** (P^{\dagger})_{i,n1}$

In[254]:=
```
2 ** (P†)_{j,m} ** P_{i,n} ** P_{j,m} //. clean
```
Out[254]=
```
2 (P†)_{j,m} ** P_{i,n} ** P_{j,m}
```
In[255]:=
```
(P†)_{j,m} ** P_{i,n} ** δ_{m,n1} ** P_{i,n} ** P_{j,m} //. clean
```
Out[255]=
```
(P†)_{j,m} ** P_{i,n} ** P_{i,n} ** P_{j,m} δ_{m,n1}
```
In[256]:=
```
(P†)_{j,m} ** 7 ** P_{i,n} ** δ_{m,n1} ** P_{i,m} ** 2 ** (P†)_{j,n1} //. clean
```
Out[256]=
```
14 (P†)_{j,m} ** P_{i,n} ** P_{i,m} ** (P†)_{j,n1} δ_{m,n1}
```
In[257]:=
```
deletezero = {NonCommutativeMultiply[x__, P_{_,_}] → 0, NonCommutativeMultiply[(P†)_{_,_}] → 0,
  NonCommutativeMultiply[P_{_,_}] → 0}
```
Out[257]=
```
{x__ ** P_{_,_} → 0, NonCommutativeMultiply[(P†)_{_,_}] → 0, NonCommutativeMultiply[P_{_,_}] → 0}
```

test the above rule

In[258]:=
```
(P†)_{i,n} ** (P†)_{j,m} ** P_{i,n} ** (P†)_{j,n1} ** P_{i,m} ** (P†)_{j,n2} ** (P†)_{i,n3} /. deletezero
(* This is because NonCommutativeMultiply is flat*)
```
Out[258]=
```
0 ** (P†)_{j,n2} ** (P†)_{i,n3}
```
In[259]:=
```
(P†)_{i,n} ** (P†)_{j,m} /. deletezero
```
Out[259]=
```
0 ** (P†)_{j,m}
```
In[260]:=
```
Replace[(P†)_{i,n} ** (P†)_{j,m} ** P_{i,n}, deletezero, {0}]
```
Out[260]=
```
0
```
In[261]:=
```
NonCommutativeMultiply[(P†)_{i,m}] /. deletezero
```
Out[261]=
```
0
```

Clearly, the above substitution rule doesn't produce the result we want. Let's try to restrict the rule to be applied only in the first level

In[262]:= $\text{Replace}\left[(P^\dagger)_{i,n} ** (P^\dagger)_{j,m} ** P_{i,n} ** (P^\dagger)_{j,n1} ** P_{i,m} ** (P^\dagger)_{j,n2} ** (P^\dagger)_{i,n3}, \text{deletezero}, \{0, 1\}\right]$

Out[262]= $(P^\dagger)_{i,n} ** (P^\dagger)_{j,m} ** P_{i,n} ** (P^\dagger)_{j,n1} ** P_{i,m} ** (P^\dagger)_{j,n2} ** (P^\dagger)_{i,n3}$

In[263]:= $\text{Replace}\left[4 (P^\dagger)_{i,n} ** (P^\dagger)_{j,n} ** (P^\dagger)_{i,n} ** P_{j,n} \epsilon_0 \delta_{n,m} \delta_{n,n1} \delta_{n,n2} C_{n1,n2,n3}, \text{deletezero}, \{0, 1\}\right]$

Out[263]= 0

In[264]:= $\text{Replace}\left[4 (P^\dagger)_{i,n} ** (P^\dagger)_{j,n} ** (P^\dagger)_{i,n} ** P_{j,n} \epsilon_0 \delta_{n,m} \delta_{n,n1} \delta_{n,n2} C_{n1,n2,n3} + (P^\dagger)_{i,n} ** (P^\dagger)_{j,m} ** P_{i,n} ** (P^\dagger)_{j,n1} ** P_{i,m} ** (P^\dagger)_{j,n2} ** (P^\dagger)_{i,n3}, \text{deletezero}, \{0, 1\}\right]$

Out[264]= $(P^\dagger)_{i,n} ** (P^\dagger)_{j,m} ** P_{i,n} ** (P^\dagger)_{j,n1} ** P_{i,m} ** (P^\dagger)_{j,n2} ** (P^\dagger)_{i,n3} + 4 (P^\dagger)_{i,n} ** (P^\dagger)_{j,n} ** (P^\dagger)_{i,n} ** P_{j,n} \epsilon_0 \delta_{n,m} \delta_{n,n1} \delta_{n,n2} C_{n1,n2,n3}$

Base on the above, deletezero can only be applied to a single term, where this single term can only have mutlitplication and noncomutative multiplications.

Let's use a module to do the above

In[265]:=
```
(* deleter terms which are zero in an expression *)
deleteZeroTerm[x_] := Module[
  {xlist, k},
  xlist = x;
  If[
   Head[xlist] === Plus,

   xlist = Apply[List, x] ; (*divide a single term into a list*)
   Do[
    xlist[[k]] = Replace[xlist[[k]], deletezero, {0, 1}],
    {k, 1, Length[xlist]}
   ];
   Apply[Plus, xlist],

   Replace[xlist, deletezero, {0, 1}]
  ]
 ]
```

In[266]:= $\text{deleteZeroTerm}[P_{j,n}]$

Out[266]= $P_{j,n}$

In[267]:= $\text{Replace}[\text{NonCommutativeMultiply}[P_{j,n}], \text{deletezero}, \{0, 1\}]$

Out[267]= 0

In[268]:= $P_{j,n}$ /. deletezero

Out[268]= $P_{j,n}$

In[269]:= deleteZeroTerm[
$4\,(P^\dagger)_{i,n} ** (P^\dagger)_{j,n} ** (P^\dagger)_{i,n} ** P_{j,n}$ +
NonCommutativeMultiply[$(P^\dagger)_{i,n}$] + NonCommutativeMultiply[$(P)_{i,n}$]
]

Out[269]= 0

In[270]:= deleteZeroTerm[%]

Out[270]= 0

In[271]:= % /. deletezero

Out[271]= 0

In[272]:= Replace[NonCommutativeMultiply[$P_{i,n}$], deletezero, {0, 1}]

Out[272]= 0

In[273]:= deleteZeroTerm[
$4\,(P^\dagger)_{i,n} ** (P^\dagger)_{j,n} ** (P^\dagger)_{i,n} + (P^\dagger)_{i,n} ** (P^\dagger)_{j,n} ** (P^\dagger)_{i,n} ** P_{j,n}$
]

Out[273]= $4\,(P^\dagger)_{i,n} ** (P^\dagger)_{j,n} ** (P^\dagger)_{i,n}$

In[274]:= deleteZeroTerm[$P_{j,n} ** (P^\dagger)_{i,n}$]

Out[274]= $P_{j,n} ** (P^\dagger)_{i,n}$

In[275]:=
```
deleteZeroTerm[(P†)i,n ** Pj,n ** (P†)i,n]
```

Out[275]= $(P^{\dagger})_{i,n} ** P_{j,n} ** (P^{\dagger})_{i,n}$

In[276]:=

According to G. Vektaris, JCP 101, 3031 (1994), the Pauli commutation relations is

$$P_n \left(P^{\dagger}\right)_m - (-1)^{\delta_{n,m}} \left(P^{\dagger}\right)_m P_n = \delta_{n,m}$$

However, the above form is cumbersome for derivations, so we rewrite it in an equivalent way as follows:

$$P_n \left(P^{\dagger}\right)_m = \delta_{n,m} + \left(P^{\dagger}\right)_m P_n - 2\,\delta_{n,m} \left(P^{\dagger}\right)_n P_n$$

It can be shown that when $n = m$, the above equation gives

$$P_n \left(P^{\dagger}\right)_n = 1 - \left(P^{\dagger}\right)_n P_n$$

which is the commutation rule for Fermions ($\left\{\left(P^{\dagger}\right)_{i,M},\ P_{j,N}\right\} = \delta_{i,j}\,\delta_{M,N}$), when $n \neq m$,

$$P_n \left(P^{\dagger}\right)_m = \left(P^{\dagger}\right)_m P_n$$

which is the commutation rule for Bosons ($\left[\left(P^{\dagger}\right)_{i,M},\ P_{j,N}\right] = \delta_{i,j}\,\delta_{M,N}$).

In[277]:=

The commutation relation (including kinematic interaction) between two operators can be written as

In[278]:=
```
commutationRule = P[i_, a_] ** Pdag[j_, b_] /; SameQ[i, j] →
  delta[a, b] + Pdag[i, b] ** P[i, a] + (-2) ** delta[a, b] ** Pdag[i, a] ** P[i, a]
(* writing in terms of (-2) will save us some trouble *)
(* it is better to regard all multiplication as noncommutative *)
```

Out[278]=
```
P[i_, a_] ** Pdag[j_, b_] /; i === j →
 delta[a, b] + Pdag[i, b] ** P[i, a] + (-2) ** delta[a, b] ** Pdag[i, a] ** P[i, a]
```

In[279]:=
```
derive[term_] := Module[
  {tmp},
  tmp = term;
  tmp = tmp /. commutationRule //. expand // ExpandAll;
  tmp = tmp //. clean;
  deleteZeroTerm[tmp]
 ]
```

In[280]:=

In[281]:=
```
(*Let's rewrite the total exciton hamiltonian (see "hamiltonian_for_exciton.nb")*)

(* to save writing, let's define something: *)
Pdag[i_, x_] := (P†)_{i, x};
P[i_, x_] := P_{i, x};
delta[x_, y_] := δ_{x,y};
A1[M_, i_, j_] := A1_M[i, j];
A2[M_, i_, j_] := A2_M[i, j];
B1[M_, L_, i_, j_] := B1_{M,L}[i, j];
B2[M_, L_, i_, j_] := B2_{M,L}[i, j];
B3[L_, M_, i_, j_] := B3_{L,M}[i, j];
B4[L_, M_, i_, j_] := B4_{L,M}[i, j];
B5[M_, i_, j_] := B5_M[i, j];
C1[M_, M2_, L_, i_, j_] := C1_{M,M2, L}[i, j]; (* M2 represents M' *)
C2[M_, L_, M2_, i_, j_] := C2_{M, L, M2}[i, j];
D1[M_, M2_, L_, L2_, i_, j_] := D1_{M,M2, L, L2}[i, j];
```

In[294]:=

In[295]:=
```
(*ignore all the summations*)
part1 = A1[M, i, j] P[j, M] + A2[M, i, j] Pdag[j, M]
part1p1 = P[j, M]
part1p2 = Pdag[j, M]
```

Out[295]= $P_{j,M}\, A1_M[i, j] + (P^\dagger)_{j,M}\, A2_M[i, j]$

Out[296]= $P_{j,M}$

Out[297]= $(P^\dagger)_{j,M}$

In[298]:=
```
part2 = B1[M, L, i, j] P[i, M] ** P[j, L] + B2[M, L, i, j] Pdag[i, M] ** Pdag[j, L]
part2p1 = P[i, M] ** P[j, L]
part2p2 = Pdag[i, M] ** Pdag[j, L]
```

Out[298]= $P_{i,M} ** P_{j,L}\, B1_{M,L}[i, j] + (P^\dagger)_{i,M} ** (P^\dagger)_{j,L}\, B2_{M,L}[i, j]$

Out[299]= $P_{i,M} ** P_{j,L}$

Out[300]= $(P^\dagger)_{i,M} ** (P^\dagger)_{j,L}$

In[301]:=
```
part3 = B3[L, M, i, j] P[i, M] ** Pdag[j, L] +
  B4[L, M, i, j] Pdag[i, L] ** P[i, M] + B5[M, i, j] Pdag[i, M] ** P[i, M]
part3p1 = P[i, M] ** Pdag[j, L]
part3p2 = Pdag[i, L] ** P[i, M]
part3p3 = Pdag[i, M] ** P[i, M]
```

Out[301]= $(P^\dagger)_{i,M} ** P_{i,M}\, B5_M[i, j] + P_{i,M} ** (P^\dagger)_{j,L}\, B3_{L,M}[i, j] + (P^\dagger)_{i,L} ** P_{i,M}\, B4_{L,M}[i, j]$

Out[302]= $P_{i,M} ** (P^\dagger)_{j,L}$

Out[303]= $(P^\dagger)_{i,L} ** P_{i,M}$

Out[304]= $(P^\dagger)_{i,M} ** P_{i,M}$

In[305]:=
```
part4 = C1[M, M2, L, i, j] Pdag[i, M] ** P[i, M2] ** P[j, L] +
  C2[M, L, M2, i, j] Pdag[i, M] ** P[i, M2] ** Pdag[j, L]
part4p1 = Pdag[i, M] ** P[i, M2] ** P[j, L]
part4p2 = Pdag[i, M] ** P[i, M2] ** Pdag[j, L]
```

Out[305]= $(P^\dagger)_{i,M} ** P_{i,M2} ** P_{j,L}\, C1_{M,M2,L}[i, j] + (P^\dagger)_{i,M} ** P_{i,M2} ** (P^\dagger)_{j,L}\, C2_{M,L,M2}[i, j]$

Out[306]= $(P^\dagger)_{i,M} ** P_{i,M2} ** P_{j,L}$

Out[307]= $(P^\dagger)_{i,M} ** P_{i,M2} ** (P^\dagger)_{j,L}$

In[308]:=

```
part5 = 1/2 D1[M, M2, L, L2, i, j] Pdag[i, M] ** P[i, M2] ** Pdag[j, L] ** P[j, L2]
part5p1 = Pdag[i, M] ** P[i, M2] ** Pdag[j, L] ** P[j, L2]
```

Out[308]= $\frac{1}{2} (P^{\dagger})_{i,M} ** P_{i,M2} ** (P^{\dagger})_{j,L} ** P_{j,L2}\, D1_{M,M2,L,L2}[i, j]$

Out[309]= $(P^{\dagger})_{i,M} ** P_{i,M2} ** (P^{\dagger})_{j,L} ** P_{j,L2}$

In[310]:=

```
(*reorder by putting operators associated with
 molecule i together and operators associated with j together*)
(*Note the following module only work if the term is
 composed of all operators associated with i and j *)
reorder[term_] := Module[{tmp, list, iList, jList, k},
  tmp = term;
  list = Apply[List, tmp];
  iList = {};
  jList = {};
  Do[
   If[
    list⟦k⟧⟦2⟧ === i, iList = Append[iList, list⟦k⟧ ], jList = Append[jList, list⟦k⟧ ]
   ],
   {k, 1, Length[list]}
  ];
  Apply[
   NonCommutativeMultiply,
   Flatten[{iList, jList}]
  ]
 ]

(* split operators associated with molecule i from that associated with molecule j*)
split2[term_] := Module[{tmp, list, iList, jList, k, ioperator, joperator},
  tmp = term;
  list = Apply[List, tmp];
  (* this will lead to problem if tmp is a single term like Pj,M *)
  iList = {};
  jList = {};

  Do[
   If[
    list⟦k⟧⟦2⟧ === i, iList = Append[iList, list⟦k⟧ ], jList = Append[jList, list⟦k⟧ ]
   ],
   {k, 1, Length[list]}
  ];

  Which[
```

```
    (* if there is no operators for molecule i and j, we use "0" as a place holder *)
    (iList === {}) && (jList === {}),
    {0, 0},

    (* if there is no operators for molecule i, we use "1" as a place holder *)
    (iList === {}) && (jList =!= {}),
    joperator = Apply[NonCommutativeMultiply, jList];
    {1, joperator},

    (iList =!= {}) && (jList === {}),
    ioperator = Apply[NonCommutativeMultiply, iList];
    {ioperator, 1},

    (iList =!= {}) && (jList =!= {}),
    ioperator = Apply[NonCommutativeMultiply, iList];
    joperator = Apply[NonCommutativeMultiply, jList];
    {ioperator, joperator}
   ]
   (*ioperator=Apply[NonCommutativeMultiply,iList];
   joperator=Apply[NonCommutativeMultiply,jList];
   {ioperator,joperator}*)
  ]

split[term_] := Module[{tmp},
   tmp = term;
   Which[
    (*consider the case when term=(P†)_{j,m2} or P_{j,M}*)
    (Head[tmp] === Subscript) && (tmp[[2]] === i),
    {tmp, 1},

    (Head[tmp] === Subscript) && (tmp[[2]] === j),
    {1, tmp},

    True,
    split2[tmp]
   ]
  ]
```

1. Consider the case $< \mathrm{n1}, \mathrm{m1} \mid V \mid \mathrm{n2}, \mathrm{m2} >$ where n1, m1, n2, m2 are not zero as an example

In[313]:=

```
(* because different terms in each part correspond to different summations,
it is better to do the derivation term by term *)
(* also it seems better to work only with the operators first: part1p1,
part1p2, ... , then substitute the final results into part1, part2, ... *)
(*list all the matrix elements ⟨n1|_i⟨m1|_jOperator|n2⟩_i|m2⟩_j ,
1 indicates states on the left, 2 indicates states on the right
 and n1, m1,n2,m2 are not ground states *)
leftOperators = P[i, n1] ** P[j, m1]
rightOperators = Pdag[i, n2] ** Pdag[j, m2]
hamOperators = List[part1p1, part1p2, part2p1,
  part2p2, part3p1, part3p2, part3p3, part4p1, part4p2, part5p1]
(*operators=Table[
  leftOperators**hamOperators[[k]]**rightOperators,
  {k,1,Length[hamOperators]}
 ]
*)
(operators = hamOperators) // MatrixForm
(*operators2=Map[reorder,operators]*)
omatrix = Map[split, operators];
omatrix // MatrixForm
```

Out[313]= $P_{i,n1} ** P_{j,m1}$

Out[314]= $(P^{\dagger})_{i,n2} ** (P^{\dagger})_{j,m2}$

Out[315]= $\{P_{j,M},\ (P^{\dagger})_{j,M},\ P_{i,M} ** P_{j,L},\ (P^{\dagger})_{i,M} ** (P^{\dagger})_{j,L},\ P_{i,M} ** (P^{\dagger})_{j,L},\ (P^{\dagger})_{i,L} ** P_{i,M},\ (P^{\dagger})_{i,M} ** P_{i,M},$
$(P^{\dagger})_{i,M} ** P_{i,M2} ** P_{j,L},\ (P^{\dagger})_{i,M} ** P_{i,M2} ** (P^{\dagger})_{j,L},\ (P^{\dagger})_{i,M} ** P_{i,M2} ** (P^{\dagger})_{j,L} ** P_{j,L2}\}$

Out[316]//MatrixForm=

$$\begin{pmatrix} P_{j,M} \\ (P^{\dagger})_{j,M} \\ P_{i,M} ** P_{j,L} \\ (P^{\dagger})_{i,M} ** (P^{\dagger})_{j,L} \\ P_{i,M} ** (P^{\dagger})_{j,L} \\ (P^{\dagger})_{i,L} ** P_{i,M} \\ (P^{\dagger})_{i,M} ** P_{i,M} \\ (P^{\dagger})_{i,M} ** P_{i,M2} ** P_{j,L} \\ (P^{\dagger})_{i,M} ** P_{i,M2} ** (P^{\dagger})_{j,L} \\ (P^{\dagger})_{i,M} ** P_{i,M2} ** (P^{\dagger})_{j,L} ** P_{j,L2} \end{pmatrix}$$

Out[318]//MatrixForm=

$$\begin{pmatrix} 1 & P_{j,M} \\ 1 & (P^{\dagger})_{j,M} \\ \text{NonCommutativeMultiply}[P_{i,M}] & \text{NonCommutativeMultiply}[P_{j,L}] \\ \text{NonCommutativeMultiply}[(P^{\dagger})_{i,M}] & \text{NonCommutativeMultiply}[(P^{\dagger})_{j,L}] \\ \text{NonCommutativeMultiply}[P_{i,M}] & \text{NonCommutativeMultiply}[(P^{\dagger})_{j,L}] \\ (P^{\dagger})_{i,L} ** P_{i,M} & 1 \\ (P^{\dagger})_{i,M} ** P_{i,M} & 1 \\ (P^{\dagger})_{i,M} ** P_{i,M2} & \text{NonCommutativeMultiply}[P_{j,L}] \\ (P^{\dagger})_{i,M} ** P_{i,M2} & \text{NonCommutativeMultiply}[(P^{\dagger})_{j,L}] \\ (P^{\dagger})_{i,M} ** P_{i,M2} & (P^{\dagger})_{j,L} ** P_{j,L2} \end{pmatrix}$$

In[319]:=

```
(*term is a 2-d array (or matrix)*)
reduceM[term_] :=
 Map[derive, term, {2}] /. {List[_, 0] → List[0, 0], List[0, _] → List[0, 0]}
```

In[320]:=

```
(*apply the function repeatly until the output doesn't change *)
FixedPoint[reduceM, omatrix] // MatrixForm
```

Out[320]//MatrixForm=

$$\begin{pmatrix} 1 & P_{j,M} \\ 1 & (P^{\dagger})_{j,M} \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \end{pmatrix}$$

2. Consider the general case $< n1, m1 \mid V \mid n2, m2 >$ where n1, m1, n2, m2 all can be zero

In[321]:=

```
(* some special case may occur *)
finalclean = {NonCommutativeMultiply[(P†)_,_, (P†)_,_] → 0, (P†)_,_ → 0, P_,_ → 0}
hamOperators1 = List[part1p1, part1p2, part2p1,
  part2p2, part3p1, part3p2, part3p3, part4p1, part4p2, part5p1]
(* the above operators doesn't consider all the cases,
by exchanging the index i and j, we can obtain other missing cases *)
hamOperators2 = hamOperators /. {i → j, j → i}
(* for the case where there is only operators associated with molecule i or j,
the above substitution will lead to problems *)
(* let's get rid of the related problems*)

(* test if an operator belongs to i or j*)
belongToi[term_] := If[term[[2]] === i, 1, 0];
belongToj[term_] := If[term[[2]] === j, 1, 0];


deleteExtraOperator[term_] := Module[
  {inum, jnum, olist},
  If[
   Head[term] === Subscript, (*if term = P_{j,M} or (P†)_{i,L}*)
   0,

   (* if the term has two or more operators *)
   olist = Apply[List, term];
   inum = Apply[
     Plus,
      Map[belongToi, olist]
    ];
   jnum = Apply[
     Plus,
      Map[belongToj, olist]
    ];
   If[(inum === 0) || (jnum === 0), 0, term]
  ]
 ]

(*hamOperators2=Map[deleteExtraOperator,hamOperators2]*)

(*left operators list*)
lolist = {P[i, n1] ** P[j, m1], P[i, n1], P[j, m1], 1}
(* bra *)
bralist = {"⟨n1|_i⟨m1|_j", "⟨n1|_i⟨0|_j", "⟨0|_i⟨m1|_j", "⟨0|_i⟨0|_j" }

(*right operators list*)
rolist = {Pdag[i, n2] ** Pdag[j, m2], Pdag[i, n2], Pdag[j, m2], 1}
(* ket *)
ketlist = {"|n2⟩_i|m2⟩_j", "|n2⟩_i|0⟩_j", "|0⟩_i|m2⟩_j", "|0⟩_i|0⟩_j" }
```

Out[321]= $\left\{(P^\dagger)_{\_,\_} ** (P^\dagger)_{\_,\_} \to 0,\ (P^\dagger)_{\_,\_} \to 0,\ P_{\_,\_} \to 0\right\}$

Out[322]= $\left\{P_{j,M},\ (P^\dagger)_{j,M},\ P_{i,M} ** P_{j,L},\ (P^\dagger)_{i,M} ** (P^\dagger)_{j,L},\ P_{i,M} ** (P^\dagger)_{j,L},\ (P^\dagger)_{i,L} ** P_{i,M},\ (P^\dagger)_{i,M} ** P_{i,M},\ (P^\dagger)_{i,M} ** P_{i,M2} ** P_{j,L},\ (P^\dagger)_{i,M} ** P_{i,M2} ** (P^\dagger)_{j,L},\ (P^\dagger)_{i,M} ** P_{i,M2} ** (P^\dagger)_{j,L} ** P_{j,L2}\right\}$

Out[323]= $\left\{P_{i,M},\ (P^\dagger)_{i,M},\ P_{j,M} ** P_{i,L},\ (P^\dagger)_{j,M} ** (P^\dagger)_{i,L},\ P_{j,M} ** (P^\dagger)_{i,L},\ (P^\dagger)_{j,L} ** P_{j,M},\ (P^\dagger)_{j,M} ** P_{j,M},\ (P^\dagger)_{j,M} ** P_{j,M2} ** P_{i,L},\ (P^\dagger)_{j,M} ** P_{j,M2} ** (P^\dagger)_{i,L},\ (P^\dagger)_{j,M} ** P_{j,M2} ** (P^\dagger)_{i,L} ** P_{i,L2}\right\}$

Out[327]= $\{P_{i,n1} ** P_{j,m1},\ P_{i,n1},\ P_{j,m1},\ 1\}$

Out[328]= $\{\langle n1|_i \langle m1|_j,\ \langle n1|_i \langle 0|_j,\ \langle 0|_i \langle m1|_j,\ \langle 0|_i \langle 0|_j\}$

Out[329]= $\{(P^\dagger)_{i,n2} ** (P^\dagger)_{j,m2},\ (P^\dagger)_{i,n2},\ (P^\dagger)_{j,m2},\ 1\}$

Out[330]= $\{|n2\rangle_i |m2\rangle_j,\ |n2\rangle_i |0\rangle_j,\ |0\rangle_i |m2\rangle_j,\ |0\rangle_i |0\rangle_j\}$

In[331]:=
```
Map[split, hamOperators2]
```

Out[331]= $\{\{P_{i,M}, 1\}, \{(P^\dagger)_{i,M}, 1\}, \{\text{NonCommutativeMultiply}[P_{i,L}], \text{NonCommutativeMultiply}[P_{j,M}]\},$
$\{\text{NonCommutativeMultiply}[(P^\dagger)_{i,L}], \text{NonCommutativeMultiply}[(P^\dagger)_{j,M}]\},$
$\{\text{NonCommutativeMultiply}[(P^\dagger)_{i,L}], \text{NonCommutativeMultiply}[P_{j,M}]\}, \{1, (P^\dagger)_{j,L} ** P_{j,M}\},$
$\{1, (P^\dagger)_{j,M} ** P_{j,M}\}, \{\text{NonCommutativeMultiply}[P_{i,L}], (P^\dagger)_{j,M} ** P_{j,M2}\},$
$\{\text{NonCommutativeMultiply}[(P^\dagger)_{i,L}], (P^\dagger)_{j,M} ** P_{j,M2}\}, \{(P^\dagger)_{i,L} ** P_{i,L2}, (P^\dagger)_{j,M} ** P_{j,M2}\}\}$

In[332]:=
```
(ham = Table[0, {x, 1, Length[lolist]}, {y, 1, Length[rolist]}]) // MatrixForm
```

Out[332]//MatrixForm=
$$\begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}$$

In[333]:=
```
(braketmat = Table[0, {x, 1, Length[lolist]}, {y, 1, Length[rolist]}]) // MatrixForm
```

Out[333]//MatrixForm=
$$\begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}$$

In[334]:=
```
Do[
 Do[
  leftOperators = lolist⟦lindex⟧;
  bra = bralist⟦lindex⟧;
  rightOperators = rolist⟦rindex⟧;
  ket = ketlist⟦rindex⟧;
  Print[
   "*******************************************************************************"];
  Print["bra state:    ", leftOperators];
  Print["ket state:    ", rightOperators];
  Print[bra <> " V " <> ket];

  operators1 =
```

```
 Which[

  (leftOperators === 1) && (rightOperators =!= 1),
  Table[
   hamOperators1[[k]] ** rightOperators,
   {k, 1, Length[hamOperators1]}
  ],

  (leftOperators =!= 1) && (rightOperators === 1),
  Table[
   leftOperators ** hamOperators1[[k]],
   {k, 1, Length[hamOperators1]}
  ],

  (leftOperators === 1) && (rightOperators === 1),
  hamOperators1,

  (leftOperators =!= 1) && (rightOperators =!= 1),
  Table[
   leftOperators ** hamOperators1[[k]] ** rightOperators, {k, 1, Length[hamOperators1]}
  ]
 ];

operators2 =
 Which[
  (leftOperators === 1) && (rightOperators =!= 1),
  Table[
   hamOperators2[[k]] ** rightOperators,
   {k, 1, Length[hamOperators2]}
  ],

  (leftOperators =!= 1) && (rightOperators === 1),
  Table[
   leftOperators ** hamOperators2[[k]],
   {k, 1, Length[hamOperators2]}
  ],

  (leftOperators === 1) && (rightOperators === 1),
  hamOperators2,

  (leftOperators =!= 1) && (rightOperators =!= 1),
  Table[
   leftOperators ** hamOperators2[[k]] ** rightOperators, {k, 1, Length[hamOperators2]}
  ]
 ];

Print["matrix elements:"];
Print[operators1];
Print["Plus"];
(* to remove the operators like P**0**P..., otherwise it will cause problems *)
operators2 = operators2 //. clean;
```

```
  Print[operators2];
  Print[" "];

  omatrix1 = Map[split, operators1];
  mat1 = FixedPoint[reduceM, omatrix1];

  omatrix2 = Map[split, operators2];
  mat2 = FixedPoint[reduceM, omatrix2];

  Print[mat1 // MatrixForm, "  +  ", mat2 // MatrixForm];
  Print[" "];
  Print["Final cleaning"];
  mat1 = mat1 /. finalclean;
  (*Print[mat1//MatrixForm];*)

  mat2 = mat2 /. finalclean;
  (*Print[mat2//MatrixForm];*)
  Print[mat1 // MatrixForm, "  +  ", mat2 // MatrixForm];

  Print[];
  matelement1 = mat1 /. {x_, y_} :→ x * y;
  matelement2 = mat2 /. {x_, y_} :→ x * y;
  matelement = matelement1 + matelement2;
  Print[matelement];
  (* save all the matrix elements *)
  ham[[lindex, rindex]] = matelement;
  braketmat[[lindex, rindex]] = bra <> " V " <> ket;

  Print[" "];
  Print[" "];
  Print[" "];
  Print[" "],
  {lindex, 1, Length[lolist]}
 ],
 {rindex, 1, Length[rolist]}
]
```

****

bra state: $P_{i,n1} ** P_{j,m1}$

ket state: $(P^\dagger)_{i,n2} ** (P^\dagger)_{j,m2}$

$\langle n1|_i \langle m1|_j \;V\; |n2\rangle_i |m2\rangle_j$

matrix elements:

$\{P_{i,n1} ** P_{j,m1} ** P_{j,M} ** (P^\dagger)_{i,n2} ** (P^\dagger)_{j,m2},$
$P_{i,n1} ** P_{j,m1} ** (P^\dagger)_{j,M} ** (P^\dagger)_{i,n2} ** (P^\dagger)_{j,m2}, P_{i,n1} ** P_{j,m1} ** P_{i,M} ** P_{j,L} ** (P^\dagger)_{i,n2} ** (P^\dagger)_{j,m2},$
$P_{i,n1} ** P_{j,m1} ** (P^\dagger)_{i,M} ** (P^\dagger)_{j,L} ** (P^\dagger)_{i,n2} ** (P^\dagger)_{j,m2}, P_{i,n1} ** P_{j,m1} ** P_{i,M} ** (P^\dagger)_{j,L} ** (P^\dagger)_{i,n2} ** (P^\dagger)_{j,m2},$
$P_{i,n1} ** P_{j,m1} ** (P^\dagger)_{i,L} ** P_{i,M} ** (P^\dagger)_{i,n2} ** (P^\dagger)_{j,m2}, P_{i,n1} ** P_{j,m1} ** (P^\dagger)_{i,M} ** P_{i,M} ** (P^\dagger)_{i,n2} ** (P^\dagger)_{j,m2},$
$P_{i,n1} ** P_{j,m1} ** (P^\dagger)_{i,M} ** P_{i,M2} ** P_{j,L} ** (P^\dagger)_{i,n2} ** (P^\dagger)_{j,m2},$
$P_{i,n1} ** P_{j,m1} ** (P^\dagger)_{i,M} ** P_{i,M2} ** (P^\dagger)_{j,L} ** (P^\dagger)_{i,n2} ** (P^\dagger)_{j,m2},$
$P_{i,n1} ** P_{j,m1} ** (P^\dagger)_{i,M} ** P_{i,M2} ** (P^\dagger)_{j,L} ** P_{j,L2} ** (P^\dagger)_{i,n2} ** (P^\dagger)_{j,m2}\}$

Plus

$$\{P_{i,n1} ** P_{j,m1} ** P_{i,M} ** (P^\dagger)_{i,n2} ** (P^\dagger)_{j,m2},$$
$$P_{i,n1} ** P_{j,m1} ** (P^\dagger)_{i,M} ** (P^\dagger)_{i,n2} ** (P^\dagger)_{j,m2},\ P_{i,n1} ** P_{j,m1} ** P_{j,M} ** P_{i,L} ** (P^\dagger)_{i,n2} ** (P^\dagger)_{j,m2},$$
$$P_{i,n1} ** P_{j,m1} ** (P^\dagger)_{j,M} ** (P^\dagger)_{i,L} ** (P^\dagger)_{i,n2} ** (P^\dagger)_{j,m2},\ P_{i,n1} ** P_{j,m1} ** P_{j,M} ** (P^\dagger)_{i,L} ** (P^\dagger)_{i,n2} ** (P^\dagger)_{j,m2},$$
$$P_{i,n1} ** P_{j,m1} ** (P^\dagger)_{j,L} ** P_{j,M} ** (P^\dagger)_{i,n2} ** (P^\dagger)_{j,m2},\ P_{i,n1} ** P_{j,m1} ** (P^\dagger)_{j,M} ** P_{j,M} ** (P^\dagger)_{i,n2} ** (P^\dagger)_{j,m2},$$
$$P_{i,n1} ** P_{j,m1} ** (P^\dagger)_{j,M} ** P_{j,M2} ** P_{i,L} ** (P^\dagger)_{i,n2} ** (P^\dagger)_{j,m2},$$
$$P_{i,n1} ** P_{j,m1} ** (P^\dagger)_{j,M} ** P_{j,M2} ** (P^\dagger)_{i,L} ** (P^\dagger)_{i,n2} ** (P^\dagger)_{j,m2},$$
$$P_{i,n1} ** P_{j,m1} ** (P^\dagger)_{j,M} ** P_{j,M2} ** (P^\dagger)_{i,L} ** P_{i,L2} ** (P^\dagger)_{i,n2} ** (P^\dagger)_{j,m2}\}$$

$$\begin{pmatrix} 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ \delta_{M,n2}\,\delta_{n1,L} & \delta_{m1,m2} \\ \delta_{M,n2}\,\delta_{n1,M} & \delta_{m1,m2} \\ 0 & 0 \\ 0 & 0 \\ \delta_{M2,n2}\,\delta_{n1,M} & \delta_{L2,m2}\,\delta_{m1,L} \end{pmatrix} + \begin{pmatrix} 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ \delta_{n1,n2} & \delta_{M,m2}\,\delta_{m1,L} \\ \delta_{n1,n2} & \delta_{M,m2}\,\delta_{m1,M} \\ 0 & 0 \\ 0 & 0 \\ \delta_{L2,n2}\,\delta_{n1,L} & \delta_{m1,M}\,\delta_{M2,m2} \end{pmatrix}$$

Final cleaning

$$\begin{pmatrix} 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ \delta_{M,n2}\,\delta_{n1,L} & \delta_{m1,m2} \\ \delta_{M,n2}\,\delta_{n1,M} & \delta_{m1,m2} \\ 0 & 0 \\ 0 & 0 \\ \delta_{M2,n2}\,\delta_{n1,M} & \delta_{L2,m2}\,\delta_{m1,L} \end{pmatrix} + \begin{pmatrix} 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ \delta_{n1,n2} & \delta_{M,m2}\,\delta_{m1,L} \\ \delta_{n1,n2} & \delta_{M,m2}\,\delta_{m1,M} \\ 0 & 0 \\ 0 & 0 \\ \delta_{L2,n2}\,\delta_{n1,L} & \delta_{m1,M}\,\delta_{M2,m2} \end{pmatrix}$$

$$\{0, 0, 0, 0, 0, \delta_{M,n2}\,\delta_{m1,m2}\,\delta_{n1,L} + \delta_{M,m2}\,\delta_{m1,L}\,\delta_{n1,n2},$$
$$\delta_{M,n2}\,\delta_{m1,m2}\,\delta_{n1,M} + \delta_{M,m2}\,\delta_{m1,M}\,\delta_{n1,n2}, 0, 0, \delta_{L2,n2}\,\delta_{m1,M}\,\delta_{M2,m2}\,\delta_{n1,L} + \delta_{L2,m2}\,\delta_{m1,L}\,\delta_{M2,n2}\,\delta_{n1,M}\}$$

****

bra state: $P_{i,n1}$

ket state: $(P^\dagger)_{i,n2} ** (P^\dagger)_{j,m2}$

$\langle n1|_i \langle 0|_j\ V\ |n2\rangle_i |m2\rangle_j$

matrix elements:

$$\{P_{i,n1} ** P_{j,M} ** (P^\dagger)_{i,n2} ** (P^\dagger)_{j,m2},\ P_{i,n1} ** (P^\dagger)_{j,M} ** (P^\dagger)_{i,n2} ** (P^\dagger)_{j,m2},$$
$$P_{i,n1} ** P_{i,M} ** P_{j,L} ** (P^\dagger)_{i,n2} ** (P^\dagger)_{j,m2},\ P_{i,n1} ** (P^\dagger)_{i,M} ** (P^\dagger)_{j,L} ** (P^\dagger)_{i,n2} ** (P^\dagger)_{j,m2},$$
$$P_{i,n1} ** P_{i,M} ** (P^\dagger)_{j,L} ** (P^\dagger)_{i,n2} ** (P^\dagger)_{j,m2},\ P_{i,n1} ** (P^\dagger)_{i,L} ** P_{i,M} ** (P^\dagger)_{i,n2} ** (P^\dagger)_{j,m2},$$
$$P_{i,n1} ** (P^\dagger)_{i,M} ** P_{i,M} ** (P^\dagger)_{i,n2} ** (P^\dagger)_{j,m2},\ P_{i,n1} ** (P^\dagger)_{i,M} ** P_{i,M2} ** P_{j,L} ** (P^\dagger)_{i,n2} ** (P^\dagger)_{j,m2},$$
$$P_{i,n1} ** (P^\dagger)_{i,M} ** P_{i,M2} ** (P^\dagger)_{j,L} ** (P^\dagger)_{i,n2} ** (P^\dagger)_{j,m2},$$
$$P_{i,n1} ** (P^\dagger)_{i,M} ** P_{i,M2} ** (P^\dagger)_{j,L} ** P_{j,L2} ** (P^\dagger)_{i,n2} ** (P^\dagger)_{j,m2}\}$$

Plus

$$\{P_{i,n1} ** P_{i,M} ** (P^\dagger)_{i,n2} ** (P^\dagger)_{j,m2},\ P_{i,n1} ** (P^\dagger)_{i,M} ** (P^\dagger)_{i,n2} ** (P^\dagger)_{j,m2},$$
$$P_{i,n1} ** P_{j,M} ** P_{i,L} ** (P^\dagger)_{i,n2} ** (P^\dagger)_{j,m2},\ P_{i,n1} ** (P^\dagger)_{j,M} ** (P^\dagger)_{i,L} ** (P^\dagger)_{i,n2} ** (P^\dagger)_{j,m2},$$
$$P_{i,n1} ** P_{j,M} ** (P^\dagger)_{i,L} ** (P^\dagger)_{i,n2} ** (P^\dagger)_{j,m2},\ P_{i,n1} ** (P^\dagger)_{j,L} ** P_{j,M} ** (P^\dagger)_{i,n2} ** (P^\dagger)_{j,m2},$$
$$P_{i,n1} ** (P^\dagger)_{j,M} ** P_{j,M} ** (P^\dagger)_{i,n2} ** (P^\dagger)_{j,m2},\ P_{i,n1} ** (P^\dagger)_{j,M} ** P_{j,M2} ** P_{i,L} ** (P^\dagger)_{i,n2} ** (P^\dagger)_{j,m2},$$
$$P_{i,n1} ** (P^\dagger)_{j,M} ** P_{j,M2} ** (P^\dagger)_{i,L} ** (P^\dagger)_{i,n2} ** (P^\dagger)_{j,m2},$$
$$P_{i,n1} ** (P^\dagger)_{j,M} ** P_{j,M2} ** (P^\dagger)_{i,L} ** P_{i,L2} ** (P^\dagger)_{i,n2} ** (P^\dagger)_{j,m2}\}$$

$$\begin{pmatrix} \delta_{n1,n2} & \delta_{M,m2} \\ \delta_{n1,n2} & (P^\dagger)_{j,M} ** (P^\dagger)_{j,m2} \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ \delta_{M2,n2}\,\delta_{n1,M} & \delta_{L,m2} \\ \delta_{M2,n2}\,\delta_{n1,M} & (P^\dagger)_{j,L} ** (P^\dagger)_{j,m2} \\ 0 & 0 \end{pmatrix} + \begin{pmatrix} 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \end{pmatrix}$$

Final cleaning

$$\begin{pmatrix} \delta_{n1,n2} & \delta_{M,m2} \\ \delta_{n1,n2} & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ \delta_{M2,n2}\,\delta_{n1,M} & \delta_{L,m2} \\ \delta_{M2,n2}\,\delta_{n1,M} & 0 \\ 0 & 0 \end{pmatrix} + \begin{pmatrix} 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \end{pmatrix}$$

$$\{\delta_{M,m2}\,\delta_{n1,n2},\ 0,\ 0,\ 0,\ 0,\ 0,\ 0,\ \delta_{L,m2}\,\delta_{M2,n2}\,\delta_{n1,M},\ 0,\ 0\}$$

****

bra state: $P_{j,m1}$

ket state: $(P^{\dagger})_{i,n2} ** (P^{\dagger})_{j,m2}$

$\langle 0|_i \langle m1|_j\ V\ |n2\rangle_i |m2\rangle_j$

matrix elements:

$$\{P_{j,m1} ** P_{j,M} ** (P^{\dagger})_{i,n2} ** (P^{\dagger})_{j,m2},\ P_{j,m1} ** (P^{\dagger})_{j,M} ** (P^{\dagger})_{i,n2} ** (P^{\dagger})_{j,m2},$$
$$P_{j,m1} ** P_{i,M} ** P_{j,L} ** (P^{\dagger})_{i,n2} ** (P^{\dagger})_{j,m2},\ P_{j,m1} ** (P^{\dagger})_{i,M} ** (P^{\dagger})_{j,L} ** (P^{\dagger})_{i,n2} ** (P^{\dagger})_{j,m2},$$
$$P_{j,m1} ** P_{i,M} ** (P^{\dagger})_{j,L} ** (P^{\dagger})_{i,n2} ** (P^{\dagger})_{j,m2},\ P_{j,m1} ** (P^{\dagger})_{i,L} ** P_{i,M} ** (P^{\dagger})_{i,n2} ** (P^{\dagger})_{j,m2},$$
$$P_{j,m1} ** (P^{\dagger})_{i,M} ** P_{i,M} ** (P^{\dagger})_{i,n2} ** (P^{\dagger})_{j,m2},\ P_{j,m1} ** (P^{\dagger})_{i,M} ** P_{i,M2} ** P_{j,L} ** (P^{\dagger})_{i,n2} ** (P^{\dagger})_{j,m2},$$
$$P_{j,m1} ** (P^{\dagger})_{i,M} ** P_{i,M2} ** (P^{\dagger})_{j,L} ** (P^{\dagger})_{i,n2} ** (P^{\dagger})_{j,m2},$$
$$P_{j,m1} ** (P^{\dagger})_{i,M} ** P_{i,M2} ** (P^{\dagger})_{j,L} ** P_{j,L2} ** (P^{\dagger})_{i,n2} ** (P^{\dagger})_{j,m2}\}$$

Plus

$$\{P_{j,m1} ** P_{i,M} ** (P^{\dagger})_{i,n2} ** (P^{\dagger})_{j,m2},\ P_{j,m1} ** (P^{\dagger})_{i,M} ** (P^{\dagger})_{i,n2} ** (P^{\dagger})_{j,m2},$$
$$P_{j,m1} ** P_{j,M} ** P_{i,L} ** (P^{\dagger})_{i,n2} ** (P^{\dagger})_{j,m2},\ P_{j,m1} ** (P^{\dagger})_{j,M} ** (P^{\dagger})_{i,L} ** (P^{\dagger})_{i,n2} ** (P^{\dagger})_{j,m2},$$
$$P_{j,m1} ** P_{j,M} ** (P^{\dagger})_{i,L} ** (P^{\dagger})_{i,n2} ** (P^{\dagger})_{j,m2},\ P_{j,m1} ** (P^{\dagger})_{j,L} ** P_{j,M} ** (P^{\dagger})_{i,n2} ** (P^{\dagger})_{j,m2},$$
$$P_{j,m1} ** (P^{\dagger})_{j,M} ** P_{j,M} ** (P^{\dagger})_{i,n2} ** (P^{\dagger})_{j,m2},\ P_{j,m1} ** (P^{\dagger})_{j,M} ** P_{j,M2} ** P_{i,L} ** (P^{\dagger})_{i,n2} ** (P^{\dagger})_{j,m2},$$
$$P_{j,m1} ** (P^{\dagger})_{j,M} ** P_{j,M2} ** (P^{\dagger})_{i,L} ** (P^{\dagger})_{i,n2} ** (P^{\dagger})_{j,m2},$$
$$P_{j,m1} ** (P^{\dagger})_{j,M} ** P_{j,M2} ** (P^{\dagger})_{i,L} ** P_{i,L2} ** (P^{\dagger})_{i,n2} ** (P^{\dagger})_{j,m2}\}$$

$$\begin{pmatrix} 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \end{pmatrix} + \begin{pmatrix} \delta_{M,n2} & \delta_{m1,m2} \\ (P^{\dagger})_{i,M} ** (P^{\dagger})_{i,n2} & \delta_{m1,m2} \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ \delta_{L,n2} & \delta_{m1,M}\,\delta_{M2,m2} \\ (P^{\dagger})_{i,L} ** (P^{\dagger})_{i,n2} & \delta_{m1,M}\,\delta_{M2,m2} \\ 0 & 0 \end{pmatrix}$$

Final cleaning

$$\begin{pmatrix} 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \end{pmatrix} + \begin{pmatrix} \delta_{M,n2} & \delta_{m1,m2} \\ 0 & \delta_{m1,m2} \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ \delta_{L,n2} & \delta_{m1,M}\,\delta_{M2,m2} \\ 0 & \delta_{m1,M}\,\delta_{M2,m2} \\ 0 & 0 \end{pmatrix}$$

$\{\delta_{M,n2}\,\delta_{m1,m2},\ 0,\ 0,\ 0,\ 0,\ 0,\ 0,\ \delta_{L,n2}\,\delta_{m1,M}\,\delta_{M2,m2},\ 0,\ 0\}$

****

bra state: 1

ket state: $(P^\dagger)_{i,n2} ** (P^\dagger)_{j,m2}$

$\langle 0|_i \langle 0|_j\ V\ |n2\rangle_i |m2\rangle_j$

matrix elements:

$\{P_{j,M} ** (P^\dagger)_{i,n2} ** (P^\dagger)_{j,m2},\ (P^\dagger)_{j,M} ** (P^\dagger)_{i,n2} ** (P^\dagger)_{j,m2},$
$P_{i,M} ** P_{j,L} ** (P^\dagger)_{i,n2} ** (P^\dagger)_{j,m2},\ (P^\dagger)_{i,M} ** (P^\dagger)_{j,L} ** (P^\dagger)_{i,n2} ** (P^\dagger)_{j,m2},$
$P_{i,M} ** (P^\dagger)_{j,L} ** (P^\dagger)_{i,n2} ** (P^\dagger)_{j,m2},\ (P^\dagger)_{i,L} ** P_{i,M} ** (P^\dagger)_{i,n2} ** (P^\dagger)_{j,m2},$
$(P^\dagger)_{i,M} ** P_{i,M} ** (P^\dagger)_{i,n2} ** (P^\dagger)_{j,m2},\ (P^\dagger)_{i,M} ** P_{i,M2} ** P_{j,L} ** (P^\dagger)_{i,n2} ** (P^\dagger)_{j,m2},$
$(P^\dagger)_{i,M} ** P_{i,M2} ** (P^\dagger)_{j,L} ** (P^\dagger)_{i,n2} ** (P^\dagger)_{j,m2},\ (P^\dagger)_{i,M} ** P_{i,M2} ** (P^\dagger)_{j,L} ** P_{j,L2} ** (P^\dagger)_{i,n2} ** (P^\dagger)_{j,m2}\}$

Plus

$\{P_{i,M} ** (P^\dagger)_{i,n2} ** (P^\dagger)_{j,m2},\ (P^\dagger)_{i,M} ** (P^\dagger)_{i,n2} ** (P^\dagger)_{j,m2},$
$P_{j,M} ** P_{i,L} ** (P^\dagger)_{i,n2} ** (P^\dagger)_{j,m2},\ (P^\dagger)_{j,M} ** (P^\dagger)_{i,L} ** (P^\dagger)_{i,n2} ** (P^\dagger)_{j,m2},$
$P_{j,M} ** (P^\dagger)_{i,L} ** (P^\dagger)_{i,n2} ** (P^\dagger)_{j,m2},\ (P^\dagger)_{j,L} ** P_{j,M} ** (P^\dagger)_{i,n2} ** (P^\dagger)_{j,m2},$
$(P^\dagger)_{j,M} ** P_{j,M} ** (P^\dagger)_{i,n2} ** (P^\dagger)_{j,m2},\ (P^\dagger)_{j,M} ** P_{j,M2} ** P_{i,L} ** (P^\dagger)_{i,n2} ** (P^\dagger)_{j,m2},$
$(P^\dagger)_{j,M} ** P_{j,M2} ** (P^\dagger)_{i,L} ** (P^\dagger)_{i,n2} ** (P^\dagger)_{j,m2},\ (P^\dagger)_{j,M} ** P_{j,M2} ** (P^\dagger)_{i,L} ** P_{i,L2} ** (P^\dagger)_{i,n2} ** (P^\dagger)_{j,m2}\}$

$$\begin{pmatrix} 0 & 0 \\ 0 & 0 \\ \delta_{M,n2} & \delta_{L,m2} \\ (P^\dagger)_{i,M} ** (P^\dagger)_{i,n2} & (P^\dagger)_{j,L} ** (P^\dagger)_{j,m2} \\ \delta_{M,n2} & (P^\dagger)_{j,L} ** (P^\dagger)_{j,m2} \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \end{pmatrix} + \begin{pmatrix} 0 & 0 \\ 0 & 0 \\ \delta_{L,n2} & \delta_{M,m2} \\ (P^\dagger)_{i,L} ** (P^\dagger)_{i,n2} & (P^\dagger)_{j,M} ** (P^\dagger)_{j,m2} \\ (P^\dagger)_{i,L} ** (P^\dagger)_{i,n2} & \delta_{M,m2} \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \end{pmatrix}$$

Final cleaning

$$\begin{pmatrix} 0 & 0 \\ 0 & 0 \\ \delta_{M,n2} & \delta_{L,m2} \\ 0 & 0 \\ \delta_{M,n2} & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \end{pmatrix} + \begin{pmatrix} 0 & 0 \\ 0 & 0 \\ \delta_{L,n2} & \delta_{M,m2} \\ 0 & 0 \\ 0 & \delta_{M,m2} \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \end{pmatrix}$$

$$\{0, 0, \delta_{L,n2}\,\delta_{M,m2} + \delta_{L,m2}\,\delta_{M,n2}, 0, 0, 0, 0, 0, 0, 0\}$$

****

bra state: $P_{i,n1} ** P_{j,m1}$

ket state: $(P^\dagger)_{i,n2}$

$\langle n1|_i \langle m1|_j\ V\ |n2\rangle_i |0\rangle_j$

matrix elements:

$$\{P_{i,n1} ** P_{j,m1} ** P_{j,M} ** (P^\dagger)_{i,n2},\ P_{i,n1} ** P_{j,m1} ** (P^\dagger)_{j,M} ** (P^\dagger)_{i,n2},\ P_{i,n1} ** P_{j,m1} ** P_{i,M} ** P_{j,L} ** (P^\dagger)_{i,n2},$$
$$P_{i,n1} ** P_{j,m1} ** (P^\dagger)_{i,M} ** (P^\dagger)_{j,L} ** (P^\dagger)_{i,n2},\ P_{i,n1} ** P_{j,m1} ** P_{i,M} ** (P^\dagger)_{j,L} ** (P^\dagger)_{i,n2},$$
$$P_{i,n1} ** P_{j,m1} ** (P^\dagger)_{i,L} ** P_{i,M} ** (P^\dagger)_{i,n2},\ P_{i,n1} ** P_{j,m1} ** (P^\dagger)_{i,M} ** P_{i,M} ** (P^\dagger)_{i,n2},$$
$$P_{i,n1} ** P_{j,m1} ** (P^\dagger)_{i,M} ** P_{i,M2} ** P_{j,L} ** (P^\dagger)_{i,n2},\ P_{i,n1} ** P_{j,m1} ** (P^\dagger)_{i,M} ** P_{i,M2} ** (P^\dagger)_{j,L} ** (P^\dagger)_{i,n2},$$
$$P_{i,n1} ** P_{j,m1} ** (P^\dagger)_{i,M} ** P_{i,M2} ** (P^\dagger)_{j,L} ** P_{j,L2} ** (P^\dagger)_{i,n2}\}$$

Plus

$\{P_{i,n1} ** P_{j,m1} ** P_{i,M} ** (P^\dagger)_{i,n2},\ P_{i,n1} ** P_{j,m1} ** (P^\dagger)_{i,M} ** (P^\dagger)_{i,n2},\ P_{i,n1} ** P_{j,m1} ** P_{j,M} ** P_{i,L} ** (P^\dagger)_{i,n2},$
$P_{i,n1} ** P_{j,m1} ** (P^\dagger)_{j,M} ** (P^\dagger)_{i,L} ** (P^\dagger)_{i,n2},\ P_{i,n1} ** P_{j,m1} ** P_{j,M} ** (P^\dagger)_{i,L} ** (P^\dagger)_{i,n2},$
$P_{i,n1} ** P_{j,m1} ** (P^\dagger)_{j,L} ** P_{j,M} ** (P^\dagger)_{i,n2},\ P_{i,n1} ** P_{j,m1} ** (P^\dagger)_{j,M} ** P_{j,M} ** (P^\dagger)_{i,n2},$
$P_{i,n1} ** P_{j,m1} ** (P^\dagger)_{j,M} ** P_{j,M2} ** P_{i,L} ** (P^\dagger)_{i,n2},\ P_{i,n1} ** P_{j,m1} ** (P^\dagger)_{j,M} ** P_{j,M2} ** (P^\dagger)_{i,L} ** (P^\dagger)_{i,n2},$
$P_{i,n1} ** P_{j,m1} ** (P^\dagger)_{j,M} ** P_{j,M2} ** (P^\dagger)_{i,L} ** P_{i,L2} ** (P^\dagger)_{i,n2}\}$

$$\begin{pmatrix} 0 & 0 \\ \delta_{n1,n2} & \delta_{m1,M} \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ \delta_{M2,n2}\,\delta_{n1,M} & \delta_{m1,L} \\ 0 & 0 \end{pmatrix} + \begin{pmatrix} 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \end{pmatrix}$$

Final cleaning

$$\begin{pmatrix} 0 & 0 \\ \delta_{n1,n2} & \delta_{m1,M} \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ \delta_{M2,n2}\,\delta_{n1,M} & \delta_{m1,L} \\ 0 & 0 \end{pmatrix} + \begin{pmatrix} 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \end{pmatrix}$$

$\{0,\ \delta_{m1,M}\,\delta_{n1,n2},\ 0,\ 0,\ 0,\ 0,\ 0,\ 0,\ \delta_{m1,L}\,\delta_{M2,n2}\,\delta_{n1,M},\ 0\}$

****

bra state: $P_{i,n1}$

ket state: $(P^\dagger)_{i,n2}$

$\langle n1|_i \langle 0|_j\ V\ |n2\rangle_i |0\rangle_j$

matrix elements:

$$\{P_{i,n1} ** P_{j,M} ** (P^\dagger)_{i,n2},\ P_{i,n1} ** (P^\dagger)_{j,M} ** (P^\dagger)_{i,n2},\ P_{i,n1} ** P_{i,M} ** P_{j,L} ** (P^\dagger)_{i,n2},$$
$$P_{i,n1} ** (P^\dagger)_{i,M} ** (P^\dagger)_{j,L} ** (P^\dagger)_{i,n2},\ P_{i,n1} ** P_{i,M} ** (P^\dagger)_{j,L} ** (P^\dagger)_{i,n2},\ P_{i,n1} ** (P^\dagger)_{i,L} ** P_{i,M} ** (P^\dagger)_{i,n2},$$
$$P_{i,n1} ** (P^\dagger)_{i,M} ** P_{i,M} ** (P^\dagger)_{i,n2},\ P_{i,n1} ** (P^\dagger)_{i,M} ** P_{i,M2} ** P_{j,L} ** (P^\dagger)_{i,n2},$$
$$P_{i,n1} ** (P^\dagger)_{i,M} ** P_{i,M2} ** (P^\dagger)_{j,L} ** (P^\dagger)_{i,n2},\ P_{i,n1} ** (P^\dagger)_{i,M} ** P_{i,M2} ** (P^\dagger)_{j,L} ** P_{j,L2} ** (P^\dagger)_{i,n2}\}$$

Plus

$$\{P_{i,n1} ** P_{i,M} ** (P^\dagger)_{i,n2},\ P_{i,n1} ** (P^\dagger)_{i,M} ** (P^\dagger)_{i,n2},\ P_{i,n1} ** P_{j,M} ** P_{i,L} ** (P^\dagger)_{i,n2},$$
$$P_{i,n1} ** (P^\dagger)_{j,M} ** (P^\dagger)_{i,L} ** (P^\dagger)_{i,n2},\ P_{i,n1} ** P_{j,M} ** (P^\dagger)_{i,L} ** (P^\dagger)_{i,n2},\ P_{i,n1} ** (P^\dagger)_{j,L} ** P_{j,M} ** (P^\dagger)_{i,n2},$$
$$P_{i,n1} ** (P^\dagger)_{j,M} ** P_{j,M} ** (P^\dagger)_{i,n2},\ P_{i,n1} ** (P^\dagger)_{j,M} ** P_{j,M2} ** P_{i,L} ** (P^\dagger)_{i,n2},$$
$$P_{i,n1} ** (P^\dagger)_{j,M} ** P_{j,M2} ** (P^\dagger)_{i,L} ** (P^\dagger)_{i,n2},\ P_{i,n1} ** (P^\dagger)_{j,M} ** P_{j,M2} ** (P^\dagger)_{i,L} ** P_{i,L2} ** (P^\dagger)_{i,n2}\}$$

$$\begin{pmatrix} 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ \delta_{M,n2}\,\delta_{n1,L} & 1 \\ \delta_{M,n2}\,\delta_{n1,M} & 1 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \end{pmatrix} + \begin{pmatrix} 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \end{pmatrix}$$

Final cleaning

$$\begin{pmatrix} 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ \delta_{M,n2}\,\delta_{n1,L} & 1 \\ \delta_{M,n2}\,\delta_{n1,M} & 1 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \end{pmatrix} + \begin{pmatrix} 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \end{pmatrix}$$

$$\{0,\ 0,\ 0,\ 0,\ 0,\ \delta_{M,n2}\,\delta_{n1,L},\ \delta_{M,n2}\,\delta_{n1,M},\ 0,\ 0,\ 0\}$$

****

bra state: $P_{j,m1}$

ket state: $(P^\dagger)_{i,n2}$

$\langle 0|_i \langle m1|_j\ V\ |n2\rangle_i |0\rangle_j$

matrix elements:

$$\{P_{j,m1} ** P_{j,M} ** (P^\dagger)_{i,n2},\ P_{j,m1} ** (P^\dagger)_{j,M} ** (P^\dagger)_{i,n2},\ P_{j,m1} ** P_{i,M} ** P_{j,L} ** (P^\dagger)_{i,n2},\ P_{j,m1} ** (P^\dagger)_{i,M} ** (P^\dagger)_{j,L} ** (P^\dagger)_{i,n2},\ P_{j,m1} ** P_{i,M} ** (P^\dagger)_{j,L} ** (P^\dagger)_{i,n2},\ P_{j,m1} ** (P^\dagger)_{i,L} ** P_{i,M} ** (P^\dagger)_{i,n2},\ P_{j,m1} ** (P^\dagger)_{i,M} ** P_{i,M} ** (P^\dagger)_{i,n2},\ P_{j,m1} ** (P^\dagger)_{i,M} ** P_{i,M2} ** P_{j,L} ** (P^\dagger)_{i,n2},\ P_{j,m1} ** (P^\dagger)_{i,M} ** P_{i,M2} ** (P^\dagger)_{j,L} ** (P^\dagger)_{i,n2},\ P_{j,m1} ** (P^\dagger)_{i,M} ** P_{i,M2} ** (P^\dagger)_{j,L} ** P_{j,L2} ** (P^\dagger)_{i,n2}\}$$

Plus

$$\{P_{j,m1} ** P_{i,M} ** (P^\dagger)_{i,n2},\ P_{j,m1} ** (P^\dagger)_{i,M} ** (P^\dagger)_{i,n2},\ P_{j,m1} ** P_{j,M} ** P_{i,L} ** (P^\dagger)_{i,n2},\ P_{j,m1} ** (P^\dagger)_{j,M} ** (P^\dagger)_{i,L} ** (P^\dagger)_{i,n2},\ P_{j,m1} ** P_{j,M} ** (P^\dagger)_{i,L} ** (P^\dagger)_{i,n2},\ P_{j,m1} ** (P^\dagger)_{j,L} ** P_{j,M} ** (P^\dagger)_{i,n2},\ P_{j,m1} ** (P^\dagger)_{j,M} ** P_{j,M} ** (P^\dagger)_{i,n2},\ P_{j,m1} ** (P^\dagger)_{j,M} ** P_{j,M2} ** P_{i,L} ** (P^\dagger)_{i,n2},\ P_{j,m1} ** (P^\dagger)_{j,M} ** P_{j,M2} ** (P^\dagger)_{i,L} ** (P^\dagger)_{i,n2},\ P_{j,m1} ** (P^\dagger)_{j,M} ** P_{j,M2} ** (P^\dagger)_{i,L} ** P_{i,L2} ** (P^\dagger)_{i,n2}\}$$

$$\begin{pmatrix} 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ (P^\dagger)_{i,M} ** (P^\dagger)_{i,n2} & \delta_{m1,L} \\ \delta_{M,n2} & \delta_{m1,L} \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \end{pmatrix} + \begin{pmatrix} 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ (P^\dagger)_{i,L} ** (P^\dagger)_{i,n2} & \delta_{m1,M} \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \end{pmatrix}$$

Final cleaning

$$\begin{pmatrix} 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & \delta_{m1,L} \\ \delta_{M,n2} & \delta_{m1,L} \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \end{pmatrix} + \begin{pmatrix} 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & \delta_{m1,M} \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \end{pmatrix}$$

$\{0, 0, 0, 0, \delta_{M,n2}\,\delta_{m1,L}, 0, 0, 0, 0, 0\}$

****

bra state: 1

ket state: $\left(P^\dagger\right)_{i,n2}$

$\langle 0|_i \langle 0|_j\ V\ |n2\rangle_i |0\rangle_j$

matrix elements:

$\{P_{j,M} ** \left(P^\dagger\right)_{i,n2},\ \left(P^\dagger\right)_{j,M} ** \left(P^\dagger\right)_{i,n2},\ P_{i,M} ** P_{j,L} ** \left(P^\dagger\right)_{i,n2},$
$\left(P^\dagger\right)_{i,M} ** \left(P^\dagger\right)_{j,L} ** \left(P^\dagger\right)_{i,n2},\ P_{i,M} ** \left(P^\dagger\right)_{j,L} ** \left(P^\dagger\right)_{i,n2},\ \left(P^\dagger\right)_{i,L} ** P_{i,M} ** \left(P^\dagger\right)_{i,n2},$
$\left(P^\dagger\right)_{i,M} ** P_{i,M} ** \left(P^\dagger\right)_{i,n2},\ \left(P^\dagger\right)_{i,M} ** P_{i,M2} ** P_{j,L} ** \left(P^\dagger\right)_{i,n2},$
$\left(P^\dagger\right)_{i,M} ** P_{i,M2} ** \left(P^\dagger\right)_{j,L} ** \left(P^\dagger\right)_{i,n2},\ \left(P^\dagger\right)_{i,M} ** P_{i,M2} ** \left(P^\dagger\right)_{j,L} ** P_{j,L2} ** \left(P^\dagger\right)_{i,n2}\}$

Plus

$\{P_{i,M} ** \left(P^\dagger\right)_{i,n2},\ \left(P^\dagger\right)_{i,M} ** \left(P^\dagger\right)_{i,n2},\ P_{j,M} ** P_{i,L} ** \left(P^\dagger\right)_{i,n2},$
$\left(P^\dagger\right)_{j,M} ** \left(P^\dagger\right)_{i,L} ** \left(P^\dagger\right)_{i,n2},\ P_{j,M} ** \left(P^\dagger\right)_{i,L} ** \left(P^\dagger\right)_{i,n2},\ \left(P^\dagger\right)_{j,L} ** P_{j,M} ** \left(P^\dagger\right)_{i,n2},$
$\left(P^\dagger\right)_{j,M} ** P_{j,M} ** \left(P^\dagger\right)_{i,n2},\ \left(P^\dagger\right)_{j,M} ** P_{j,M2} ** P_{i,L} ** \left(P^\dagger\right)_{i,n2},$
$\left(P^\dagger\right)_{j,M} ** P_{j,M2} ** \left(P^\dagger\right)_{i,L} ** \left(P^\dagger\right)_{i,n2},\ \left(P^\dagger\right)_{j,M} ** P_{j,M2} ** \left(P^\dagger\right)_{i,L} ** P_{i,L2} ** \left(P^\dagger\right)_{i,n2}\}$

$$\begin{pmatrix} 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \end{pmatrix} + \begin{pmatrix} \delta_{M,n2} & 1 \\ \left(P^\dagger\right)_{i,M} ** \left(P^\dagger\right)_{i,n2} & 1 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \end{pmatrix}$$

Final cleaning

$$\begin{pmatrix} 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \end{pmatrix} + \begin{pmatrix} \delta_{M,n2} & 1 \\ 0 & 1 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \end{pmatrix}$$

$\{\delta_{M,n2}, 0, 0, 0, 0, 0, 0, 0, 0, 0\}$

****

bra state: $P_{i,n1} ** P_{j,m1}$

ket state: $\left(P^{\dagger}\right)_{j,m2}$

$\langle n1|_i \langle m1|_j \; V \; |0\rangle_i |m2\rangle_j$

matrix elements:

$$\left\{P_{i,n1} ** P_{j,m1} ** P_{j,M} ** \left(P^{\dagger}\right)_{j,m2},\ P_{i,n1} ** P_{j,m1} ** \left(P^{\dagger}\right)_{j,M} ** \left(P^{\dagger}\right)_{j,m2},\ P_{i,n1} ** P_{j,m1} ** P_{i,M} ** P_{j,L} ** \left(P^{\dagger}\right)_{j,m2},\right.$$
$$P_{i,n1} ** P_{j,m1} ** \left(P^{\dagger}\right)_{i,M} ** \left(P^{\dagger}\right)_{j,L} ** \left(P^{\dagger}\right)_{j,m2},\ P_{i,n1} ** P_{j,m1} ** P_{i,M} ** \left(P^{\dagger}\right)_{j,L} ** \left(P^{\dagger}\right)_{j,m2},$$
$$P_{i,n1} ** P_{j,m1} ** \left(P^{\dagger}\right)_{i,L} ** P_{i,M} ** \left(P^{\dagger}\right)_{j,m2},\ P_{i,n1} ** P_{j,m1} ** \left(P^{\dagger}\right)_{i,M} ** P_{i,M} ** \left(P^{\dagger}\right)_{j,m2},$$
$$P_{i,n1} ** P_{j,m1} ** \left(P^{\dagger}\right)_{i,M} ** P_{i,M2} ** P_{j,L} ** \left(P^{\dagger}\right)_{j,m2},\ P_{i,n1} ** P_{j,m1} ** \left(P^{\dagger}\right)_{i,M} ** P_{i,M2} ** \left(P^{\dagger}\right)_{j,L} ** \left(P^{\dagger}\right)_{j,m2},$$
$$\left.P_{i,n1} ** P_{j,m1} ** \left(P^{\dagger}\right)_{i,M} ** P_{i,M2} ** \left(P^{\dagger}\right)_{j,L} ** P_{j,L2} ** \left(P^{\dagger}\right)_{j,m2}\right\}$$

Plus

$$\left\{P_{i,n1} ** P_{j,m1} ** P_{i,M} ** \left(P^{\dagger}\right)_{j,m2},\ P_{i,n1} ** P_{j,m1} ** \left(P^{\dagger}\right)_{i,M} ** \left(P^{\dagger}\right)_{j,m2},\ P_{i,n1} ** P_{j,m1} ** P_{j,M} ** P_{i,L} ** \left(P^{\dagger}\right)_{j,m2},\right.$$
$$P_{i,n1} ** P_{j,m1} ** \left(P^{\dagger}\right)_{j,M} ** \left(P^{\dagger}\right)_{i,L} ** \left(P^{\dagger}\right)_{j,m2},\ P_{i,n1} ** P_{j,m1} ** P_{j,M} ** \left(P^{\dagger}\right)_{i,L} ** \left(P^{\dagger}\right)_{j,m2},$$
$$P_{i,n1} ** P_{j,m1} ** \left(P^{\dagger}\right)_{j,L} ** P_{j,M} ** \left(P^{\dagger}\right)_{j,m2},\ P_{i,n1} ** P_{j,m1} ** \left(P^{\dagger}\right)_{j,M} ** P_{j,M} ** \left(P^{\dagger}\right)_{j,m2},$$
$$P_{i,n1} ** P_{j,m1} ** \left(P^{\dagger}\right)_{j,M} ** P_{j,M2} ** P_{i,L} ** \left(P^{\dagger}\right)_{j,m2},\ P_{i,n1} ** P_{j,m1} ** \left(P^{\dagger}\right)_{j,M} ** P_{j,M2} ** \left(P^{\dagger}\right)_{i,L} ** \left(P^{\dagger}\right)_{j,m2},$$
$$\left.P_{i,n1} ** P_{j,m1} ** \left(P^{\dagger}\right)_{j,M} ** P_{j,M2} ** \left(P^{\dagger}\right)_{i,L} ** P_{i,L2} ** \left(P^{\dagger}\right)_{j,m2}\right\}$$

$$\begin{pmatrix} 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \end{pmatrix} + \begin{pmatrix} 0 & 0 \\ \delta_{n1,M} & \delta_{m1,m2} \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ \delta_{n1,L} & \delta_{m1,M}\,\delta_{M2,m2} \\ 0 & 0 \end{pmatrix}$$

Final cleaning

$$\begin{pmatrix} 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \end{pmatrix} + \begin{pmatrix} 0 & 0 \\ \delta_{n1,M} & \delta_{m1,m2} \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ \delta_{n1,L} & \delta_{m1,M}\,\delta_{M2,m2} \\ 0 & 0 \end{pmatrix}$$

$\{0, \delta_{m1,m2}\,\delta_{n1,M}, 0, 0, 0, 0, 0, 0, \delta_{m1,M}\,\delta_{M2,m2}\,\delta_{n1,L}, 0\}$

****

bra state: $P_{i,n1}$

ket state: $(P^{\dagger})_{j,m2}$

$\langle n1|_i \langle 0|_j\ V\ |0\rangle_i |m2\rangle_j$

matrix elements:

$$\{P_{i,n1} ** P_{j,M} ** (P^{\dagger})_{j,m2}, P_{i,n1} ** (P^{\dagger})_{j,M} ** (P^{\dagger})_{j,m2}, P_{i,n1} ** P_{i,M} ** P_{j,L} ** (P^{\dagger})_{j,m2}, P_{i,n1} ** (P^{\dagger})_{i,M} ** (P^{\dagger})_{j,L} ** (P^{\dagger})_{j,m2}, P_{i,n1} ** P_{i,M} ** (P^{\dagger})_{j,L} ** (P^{\dagger})_{j,m2}, P_{i,n1} ** (P^{\dagger})_{i,L} ** P_{i,M} ** (P^{\dagger})_{j,m2}, P_{i,n1} ** (P^{\dagger})_{i,M} ** P_{i,M} ** (P^{\dagger})_{j,m2}, P_{i,n1} ** (P^{\dagger})_{i,M} ** P_{i,M2} ** P_{j,L} ** (P^{\dagger})_{j,m2}, P_{i,n1} ** (P^{\dagger})_{i,M} ** P_{i,M2} ** (P^{\dagger})_{j,L} ** (P^{\dagger})_{j,m2}, P_{i,n1} ** (P^{\dagger})_{i,M} ** P_{i,M2} ** (P^{\dagger})_{j,L} ** P_{j,L2} ** (P^{\dagger})_{j,m2}\}$$

Plus

$$\{P_{i,n1} ** P_{i,M} ** (P^{\dagger})_{j,m2}, P_{i,n1} ** (P^{\dagger})_{i,M} ** (P^{\dagger})_{j,m2}, P_{i,n1} ** P_{j,M} ** P_{i,L} ** (P^{\dagger})_{j,m2}, P_{i,n1} ** (P^{\dagger})_{j,M} ** (P^{\dagger})_{i,L} ** (P^{\dagger})_{j,m2}, P_{i,n1} ** P_{j,M} ** (P^{\dagger})_{i,L} ** (P^{\dagger})_{j,m2}, P_{i,n1} ** (P^{\dagger})_{j,L} ** P_{j,M} ** (P^{\dagger})_{j,m2}, P_{i,n1} ** (P^{\dagger})_{j,M} ** P_{j,M} ** (P^{\dagger})_{j,m2}, P_{i,n1} ** (P^{\dagger})_{j,M} ** P_{j,M2} ** P_{i,L} ** (P^{\dagger})_{j,m2}, P_{i,n1} ** (P^{\dagger})_{j,M} ** P_{j,M2} ** (P^{\dagger})_{i,L} ** (P^{\dagger})_{j,m2}, P_{i,n1} ** (P^{\dagger})_{j,M} ** P_{j,M2} ** (P^{\dagger})_{i,L} ** P_{i,L2} ** (P^{\dagger})_{j,m2}\}$$

$$\begin{pmatrix} 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ \delta_{n1,M} & (P^{\dagger})_{j,L} ** (P^{\dagger})_{j,m2} \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \end{pmatrix} + \begin{pmatrix} 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ \delta_{n1,L} & (P^{\dagger})_{j,M} ** (P^{\dagger})_{j,m2} \\ \delta_{n1,L} & \delta_{M,m2} \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \end{pmatrix}$$

Final cleaning

$$\begin{pmatrix} 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ \delta_{n1,M} & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \end{pmatrix} + \begin{pmatrix} 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ \delta_{n1,L} & 0 \\ \delta_{n1,L} & \delta_{M,m2} \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \end{pmatrix}$$

$\{0, 0, 0, 0, \delta_{M,m2}\,\delta_{n1,L}, 0, 0, 0, 0, 0\}$

****

bra state: $P_{j,m1}$

ket state: $(P^\dagger)_{j,m2}$

$\langle 0|_i \langle m1|_j\ V\ |0\rangle_i |m2\rangle_j$

matrix elements:

$\{P_{j,m1} ** P_{j,M} ** (P^\dagger)_{j,m2},\ P_{j,m1} ** (P^\dagger)_{j,M} ** (P^\dagger)_{j,m2},\ P_{j,m1} ** P_{i,M} ** P_{j,L} ** (P^\dagger)_{j,m2},$
$P_{j,m1} ** (P^\dagger)_{i,M} ** (P^\dagger)_{j,L} ** (P^\dagger)_{j,m2},\ P_{j,m1} ** P_{i,M} ** (P^\dagger)_{j,L} ** (P^\dagger)_{j,m2},\ P_{j,m1} ** (P^\dagger)_{i,L} ** P_{i,M} ** (P^\dagger)_{j,m2},$
$P_{j,m1} ** (P^\dagger)_{i,M} ** P_{i,M} ** (P^\dagger)_{j,m2},\ P_{j,m1} ** (P^\dagger)_{i,M} ** P_{i,M2} ** P_{j,L} ** (P^\dagger)_{j,m2},$
$P_{j,m1} ** (P^\dagger)_{i,M} ** P_{i,M2} ** (P^\dagger)_{j,L} ** (P^\dagger)_{j,m2},\ P_{j,m1} ** (P^\dagger)_{i,M} ** P_{i,M2} ** (P^\dagger)_{j,L} ** P_{j,L2} ** (P^\dagger)_{j,m2}\}$

Plus

$\{P_{j,m1} ** P_{i,M} ** (P^\dagger)_{j,m2},\ P_{j,m1} ** (P^\dagger)_{i,M} ** (P^\dagger)_{j,m2},\ P_{j,m1} ** P_{j,M} ** P_{i,L} ** (P^\dagger)_{j,m2},$
$P_{j,m1} ** (P^\dagger)_{j,M} ** (P^\dagger)_{i,L} ** (P^\dagger)_{j,m2},\ P_{j,m1} ** P_{j,M} ** (P^\dagger)_{i,L} ** (P^\dagger)_{j,m2},\ P_{j,m1} ** (P^\dagger)_{j,L} ** P_{j,M} ** (P^\dagger)_{j,m2},$
$P_{j,m1} ** (P^\dagger)_{j,M} ** P_{j,M} ** (P^\dagger)_{j,m2},\ P_{j,m1} ** (P^\dagger)_{j,M} ** P_{j,M2} ** P_{i,L} ** (P^\dagger)_{j,m2},$
$P_{j,m1} ** (P^\dagger)_{j,M} ** P_{j,M2} ** (P^\dagger)_{i,L} ** (P^\dagger)_{j,m2},\ P_{j,m1} ** (P^\dagger)_{j,M} ** P_{j,M2} ** (P^\dagger)_{i,L} ** P_{i,L2} ** (P^\dagger)_{j,m2}\}$

$$\begin{pmatrix} 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \end{pmatrix} + \begin{pmatrix} 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 1 & \delta_{M,m2}\,\delta_{m1,L} \\ 1 & \delta_{M,m2}\,\delta_{m1,M} \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \end{pmatrix}$$

Final cleaning

$$\begin{pmatrix} 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \end{pmatrix} + \begin{pmatrix} 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 1 & \delta_{M,m2}\,\delta_{m1,L} \\ 1 & \delta_{M,m2}\,\delta_{m1,M} \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \end{pmatrix}$$

$\{0, 0, 0, 0, 0, \delta_{M,m2}\,\delta_{m1,L}, \delta_{M,m2}\,\delta_{m1,M}, 0, 0, 0\}$

****

bra state: 1

ket state: $(P^\dagger)_{j,m2}$

$\langle 0|_i \langle 0|_j\ V\ |0\rangle_i |m2\rangle_j$

matrix elements:

$\{P_{j,M} ** (P^\dagger)_{j,m2}, (P^\dagger)_{j,M} ** (P^\dagger)_{j,m2}, P_{i,M} ** P_{j,L} ** (P^\dagger)_{j,m2},$
$(P^\dagger)_{i,M} ** (P^\dagger)_{j,L} ** (P^\dagger)_{j,m2}, P_{i,M} ** (P^\dagger)_{j,L} ** (P^\dagger)_{j,m2}, (P^\dagger)_{i,L} ** P_{i,M} ** (P^\dagger)_{j,m2},$
$(P^\dagger)_{i,M} ** P_{i,M} ** (P^\dagger)_{j,m2}, (P^\dagger)_{i,M} ** P_{i,M2} ** P_{j,L} ** (P^\dagger)_{j,m2},$
$(P^\dagger)_{i,M} ** P_{i,M2} ** (P^\dagger)_{j,L} ** (P^\dagger)_{j,m2}, (P^\dagger)_{i,M} ** P_{i,M2} ** (P^\dagger)_{j,L} ** P_{j,L2} ** (P^\dagger)_{j,m2}\}$

Plus

$\{P_{i,M} ** (P^\dagger)_{j,m2}, (P^\dagger)_{i,M} ** (P^\dagger)_{j,m2}, P_{j,M} ** P_{i,L} ** (P^\dagger)_{j,m2},$
$(P^\dagger)_{j,M} ** (P^\dagger)_{i,L} ** (P^\dagger)_{j,m2}, P_{j,M} ** (P^\dagger)_{i,L} ** (P^\dagger)_{j,m2}, (P^\dagger)_{j,L} ** P_{j,M} ** (P^\dagger)_{j,m2},$
$(P^\dagger)_{j,M} ** P_{j,M} ** (P^\dagger)_{j,m2}, (P^\dagger)_{j,M} ** P_{j,M2} ** P_{i,L} ** (P^\dagger)_{j,m2},$
$(P^\dagger)_{j,M} ** P_{j,M2} ** (P^\dagger)_{i,L} ** (P^\dagger)_{j,m2}, (P^\dagger)_{j,M} ** P_{j,M2} ** (P^\dagger)_{i,L} ** P_{i,L2} ** (P^\dagger)_{j,m2}\}$

$$\begin{pmatrix} 1 & \delta_{M,m2} \\ 1 & (P^\dagger)_{j,M} ** (P^\dagger)_{j,m2} \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \end{pmatrix} + \begin{pmatrix} 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \end{pmatrix}$$

Final cleaning

$$\begin{pmatrix} 1 & \delta_{M,m2} \\ 1 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \end{pmatrix} + \begin{pmatrix} 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \end{pmatrix}$$

$\{\delta_{M,m2}, 0, 0, 0, 0, 0, 0, 0, 0, 0\}$

****

bra state: $P_{i,n1} ** P_{j,m1}$

ket state: 1

$\langle n1|_i \langle m1|_j\ V\ |0\rangle_i |0\rangle_j$

matrix elements:

$$\{P_{i,n1} ** P_{j,m1} ** P_{j,M},\ P_{i,n1} ** P_{j,m1} ** (P^\dagger)_{j,M},\ P_{i,n1} ** P_{j,m1} ** P_{i,M} ** P_{j,L},$$
$$P_{i,n1} ** P_{j,m1} ** (P^\dagger)_{i,M} ** (P^\dagger)_{j,L},\ P_{i,n1} ** P_{j,m1} ** P_{i,M} ** (P^\dagger)_{j,L},\ P_{i,n1} ** P_{j,m1} ** (P^\dagger)_{i,L} ** P_{i,M},$$
$$P_{i,n1} ** P_{j,m1} ** (P^\dagger)_{i,M} ** P_{i,M},\ P_{i,n1} ** P_{j,m1} ** (P^\dagger)_{i,M} ** P_{i,M2} ** P_{j,L},$$
$$P_{i,n1} ** P_{j,m1} ** (P^\dagger)_{i,M} ** P_{i,M2} ** (P^\dagger)_{j,L},\ P_{i,n1} ** P_{j,m1} ** (P^\dagger)_{i,M} ** P_{i,M2} ** (P^\dagger)_{j,L} ** P_{j,L2}\}$$

Plus

$\{P_{i,n1} ** P_{j,m1} ** P_{i,M},\ P_{i,n1} ** P_{j,m1} ** (P^\dagger)_{i,M},\ P_{i,n1} ** P_{j,m1} ** P_{j,M} ** P_{i,L},$
$P_{i,n1} ** P_{j,m1} ** (P^\dagger)_{j,M} ** (P^\dagger)_{i,L},\ P_{i,n1} ** P_{j,m1} ** P_{j,M} ** (P^\dagger)_{i,L},\ P_{i,n1} ** P_{j,m1} ** (P^\dagger)_{j,L} ** P_{j,M},$
$P_{i,n1} ** P_{j,m1} ** (P^\dagger)_{j,M} ** P_{j,M},\ P_{i,n1} ** P_{j,m1} ** (P^\dagger)_{j,M} ** P_{j,M2} ** P_{i,L},$
$P_{i,n1} ** P_{j,m1} ** (P^\dagger)_{j,M} ** P_{j,M2} ** (P^\dagger)_{i,L},\ P_{i,n1} ** P_{j,m1} ** (P^\dagger)_{j,M} ** P_{j,M2} ** (P^\dagger)_{i,L} ** P_{i,L2}\}$

$$\begin{pmatrix} 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ \delta_{n1,M} & \delta_{m1,L} \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \end{pmatrix} + \begin{pmatrix} 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ \delta_{n1,L} & \delta_{m1,M} \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \end{pmatrix}$$

Final cleaning

$$\begin{pmatrix} 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ \delta_{n1,M} & \delta_{m1,L} \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \end{pmatrix} + \begin{pmatrix} 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ \delta_{n1,L} & \delta_{m1,M} \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \end{pmatrix}$$

$\{0, 0, 0, \delta_{m1,M}\,\delta_{n1,L} + \delta_{m1,L}\,\delta_{n1,M}, 0, 0, 0, 0, 0, 0\}$

****

bra state: $P_{i,n1}$

ket state: 1

$\langle n1|_i \langle 0|_j\ V\ |0\rangle_i |0\rangle_j$

matrix elements:

$\{P_{i,n1} ** P_{j,M},\ P_{i,n1} ** (P^\dagger)_{j,M},\ P_{i,n1} ** P_{i,M} ** P_{j,L},\ P_{i,n1} ** (P^\dagger)_{i,M} ** (P^\dagger)_{j,L},$
$P_{i,n1} ** P_{i,M} ** (P^\dagger)_{j,L},\ P_{i,n1} ** (P^\dagger)_{i,L} ** P_{i,M},\ P_{i,n1} ** (P^\dagger)_{i,M} ** P_{i,M},\ P_{i,n1} ** (P^\dagger)_{i,M} ** P_{i,M2} ** P_{j,L},$
$P_{i,n1} ** (P^\dagger)_{i,M} ** P_{i,M2} ** (P^\dagger)_{j,L},\ P_{i,n1} ** (P^\dagger)_{i,M} ** P_{i,M2} ** (P^\dagger)_{j,L} ** P_{j,L2}\}$

Plus

$\{P_{i,n1} ** P_{i,M},\ P_{i,n1} ** (P^{\dagger})_{i,M},\ P_{i,n1} ** P_{j,M} ** P_{i,L},\ P_{i,n1} ** (P^{\dagger})_{j,M} ** (P^{\dagger})_{i,L},$
$P_{i,n1} ** P_{j,M} ** (P^{\dagger})_{i,L},\ P_{i,n1} ** (P^{\dagger})_{j,L} ** P_{j,M},\ P_{i,n1} ** (P^{\dagger})_{j,M} ** P_{j,M},\ P_{i,n1} ** (P^{\dagger})_{j,M} ** P_{j,M2} ** P_{i,L},$
$P_{i,n1} ** (P^{\dagger})_{j,M} ** P_{j,M2} ** (P^{\dagger})_{i,L},\ P_{i,n1} ** (P^{\dagger})_{j,M} ** P_{j,M2} ** (P^{\dagger})_{i,L} ** P_{i,L2}\}$

$$\begin{pmatrix} 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \end{pmatrix} + \begin{pmatrix} 0 & 0 \\ \delta_{n1,M} & 1 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \end{pmatrix}$$

Final cleaning

$$\begin{pmatrix} 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \end{pmatrix} + \begin{pmatrix} 0 & 0 \\ \delta_{n1,M} & 1 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \end{pmatrix}$$

$\{0,\ \delta_{n1,M},\ 0,\ 0,\ 0,\ 0,\ 0,\ 0,\ 0,\ 0\}$

****

bra state: $P_{j,m1}$

ket state: 1

$\langle 0|_i \langle m1|_j\ V\ |0\rangle_i |0\rangle_j$

matrix elements:

$\{P_{j,m1} ** P_{j,M},\ P_{j,m1} ** (P^{\dagger})_{j,M},\ P_{j,m1} ** P_{i,M} ** P_{j,L},\ P_{j,m1} ** (P^{\dagger})_{i,M} ** (P^{\dagger})_{j,L},$
$P_{j,m1} ** P_{i,M} ** (P^{\dagger})_{j,L},\ P_{j,m1} ** (P^{\dagger})_{i,L} ** P_{i,M},\ P_{j,m1} ** (P^{\dagger})_{i,M} ** P_{i,M},\ P_{j,m1} ** (P^{\dagger})_{i,M} ** P_{i,M2} ** P_{j,L},$
$P_{j,m1} ** (P^{\dagger})_{i,M} ** P_{i,M2} ** (P^{\dagger})_{j,L},\ P_{j,m1} ** (P^{\dagger})_{i,M} ** P_{i,M2} ** (P^{\dagger})_{j,L} ** P_{j,L2}\}$

Plus

$\{P_{j,m1} ** P_{i,M},\ P_{j,m1} ** (P^{\dagger})_{i,M},\ P_{j,m1} ** P_{j,M} ** P_{i,L},\ P_{j,m1} ** (P^{\dagger})_{j,M} ** (P^{\dagger})_{i,L},$
$P_{j,m1} ** P_{j,M} ** (P^{\dagger})_{i,L},\ P_{j,m1} ** (P^{\dagger})_{j,L} ** P_{j,M},\ P_{j,m1} ** (P^{\dagger})_{j,M} ** P_{j,M},\ P_{j,m1} ** (P^{\dagger})_{j,M} ** P_{j,M2} ** P_{i,L},$
$P_{j,m1} ** (P^{\dagger})_{j,M} ** P_{j,M2} ** (P^{\dagger})_{i,L},\ P_{j,m1} ** (P^{\dagger})_{j,M} ** P_{j,M2} ** (P^{\dagger})_{i,L} ** P_{i,L2}\}$

$$\begin{pmatrix} 0 & 0 \\ 1 & \delta_{m1,M} \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \end{pmatrix} + \begin{pmatrix} 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \end{pmatrix}$$

Final cleaning

$$\begin{pmatrix} 0 & 0 \\ 1 & \delta_{m1,M} \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \end{pmatrix} + \begin{pmatrix} 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \end{pmatrix}$$

$\{0,\ \delta_{m1,M},\ 0,\ 0,\ 0,\ 0,\ 0,\ 0,\ 0,\ 0\}$

****

bra state: 1

ket state: 1

$\langle 0|_i \langle 0|_j\ V\ |0\rangle_i |0\rangle_j$

matrix elements:

$\{P_{j,M},\ (P^{\dagger})_{j,M},\ P_{i,M} ** P_{j,L},\ (P^{\dagger})_{i,M} ** (P^{\dagger})_{j,L},\ P_{i,M} ** (P^{\dagger})_{j,L},\ (P^{\dagger})_{i,L} ** P_{i,M},\ (P^{\dagger})_{i,M} ** P_{i,M},$
$(P^{\dagger})_{i,M} ** P_{i,M2} ** P_{j,L},\ (P^{\dagger})_{i,M} ** P_{i,M2} ** (P^{\dagger})_{j,L},\ (P^{\dagger})_{i,M} ** P_{i,M2} ** (P^{\dagger})_{j,L} ** P_{j,L2}\}$

Plus

$$\left\{P_{i,M},\ (P^\dagger)_{i,M},\ P_{j,M} ** P_{i,L},\ (P^\dagger)_{j,M} ** (P^\dagger)_{i,L},\ P_{j,M} ** (P^\dagger)_{i,L},\ (P^\dagger)_{j,L} ** P_{j,M},\ (P^\dagger)_{j,M} ** P_{j,M},\right.$$
$$\left.(P^\dagger)_{j,M} ** P_{j,M2} ** P_{i,L},\ (P^\dagger)_{j,M} ** P_{j,M2} ** (P^\dagger)_{i,L},\ (P^\dagger)_{j,M} ** P_{j,M2} ** (P^\dagger)_{i,L} ** P_{i,L2}\right\}$$

$$\begin{pmatrix} 1 & P_{j,M} \\ 1 & (P^\dagger)_{j,M} \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \end{pmatrix} + \begin{pmatrix} P_{i,M} & 1 \\ (P^\dagger)_{i,M} & 1 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \end{pmatrix}$$

Final cleaning

$$\begin{pmatrix} 1 & 0 \\ 1 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \end{pmatrix} + \begin{pmatrix} 0 & 1 \\ 0 & 1 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \end{pmatrix}$$

$$\{0, 0, 0, 0, 0, 0, 0, 0, 0, 0\}$$

In[335]:=
```
ham // MatrixForm
braketmat // MatrixForm
```

Out[335]//MatrixForm=

$$\begin{pmatrix}
\begin{pmatrix} 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ \delta_{M,n2}\,\delta_{m1,m2}\,\delta_{n1,L} + \delta_{M,m2}\,\delta_{m1,L}\,\delta_{n1,n2} \\ \delta_{M,n2}\,\delta_{m1,m2}\,\delta_{n1,M} + \delta_{M,m2}\,\delta_{m1,M}\,\delta_{n1,n2} \\ 0 \\ 0 \\ \delta_{L2,n2}\,\delta_{m1,M}\,\delta_{M2,m2}\,\delta_{n1,L} + \delta_{L2,m2}\,\delta_{m1,L}\,\delta_{M2,n2}\,\delta_{n1,M} \end{pmatrix} &
\begin{pmatrix} 0 \\ \delta_{m1,M}\,\delta_{n1,n2} \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ \delta_{m1,L}\,\delta_{M2,n2}\,\delta_{n1,M} \\ 0 \end{pmatrix} &
\begin{pmatrix} 0 \\ \delta_{m1,m2}\,\delta_{n1,M} \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ \delta_{m1,M}\,\delta_{M2,m2}\,\delta_{n1,L} \\ 0 \end{pmatrix} &
\begin{pmatrix} 0 \\ 0 \\ 0 \\ \delta_{m1,M}\,\delta_{n1,L} + \delta_{m1} \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \end{pmatrix} \\
\begin{pmatrix} \delta_{M,m2}\,\delta_{n1,n2} \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ \delta_{L,m2}\,\delta_{M2,n2}\,\delta_{n1,M} \\ 0 \\ 0 \end{pmatrix} &
\begin{pmatrix} 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ \delta_{M,n2}\,\delta_{n1,L} \\ \delta_{M,n2}\,\delta_{n1,M} \\ 0 \\ 0 \\ 0 \end{pmatrix} &
\begin{pmatrix} 0 \\ 0 \\ 0 \\ 0 \\ \delta_{M,m2}\,\delta_{n1,L} \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \end{pmatrix} &
\begin{pmatrix} 0 \\ \delta_{n1,M} \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \end{pmatrix} \\
\begin{pmatrix} \delta_{M,n2}\,\delta_{m1,m2} \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ \delta_{L,n2}\,\delta_{m1,M}\,\delta_{M2,m2} \\ 0 \\ 0 \end{pmatrix} &
\begin{pmatrix} 0 \\ 0 \\ 0 \\ 0 \\ \delta_{M,n2}\,\delta_{m1,L} \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \end{pmatrix} &
\begin{pmatrix} 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ \delta_{M,m2}\,\delta_{m1,L} \\ \delta_{M,m2}\,\delta_{m1,M} \\ 0 \\ 0 \\ 0 \end{pmatrix} &
\begin{pmatrix} 0 \\ \delta_{m1,M} \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \end{pmatrix} \\
\begin{pmatrix} 0 \\ 0 \\ \delta_{L,n2}\,\delta_{M,m2} + \delta_{L,m2}\,\delta_{M,n2} \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \end{pmatrix} &
\begin{pmatrix} \delta_{M,n2} \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \end{pmatrix} &
\begin{pmatrix} \delta_{M,m2} \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \end{pmatrix} &
\begin{pmatrix} 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \end{pmatrix}
\end{pmatrix}$$

Out[336]//MatrixForm=

$$\begin{pmatrix}
\langle n1|_i\langle m1|_j\ V\ |n2\rangle_i|m2\rangle_j & \langle n1|_i\langle m1|_j\ V\ |n2\rangle_i|0\rangle_j & \langle n1|_i\langle m1|_j\ V\ |0\rangle_i|m2\rangle_j & \langle n1|_i\langle m1|_j\ V\ |0\rangle_i|0\rangle_j \\
\langle n1|_i\langle 0|_j\ V\ |n2\rangle_i|m2\rangle_j & \langle n1|_i\langle 0|_j\ V\ |n2\rangle_i|0\rangle_j & \langle n1|_i\langle 0|_j\ V\ |0\rangle_i|m2\rangle_j & \langle n1|_i\langle 0|_j\ V\ |0\rangle_i|0\rangle_j \\
\langle 0|_i\langle m1|_j\ V\ |n2\rangle_i|m2\rangle_j & \langle 0|_i\langle m1|_j\ V\ |n2\rangle_i|0\rangle_j & \langle 0|_i\langle m1|_j\ V\ |0\rangle_i|m2\rangle_j & \langle 0|_i\langle m1|_j\ V\ |0\rangle_i|0\rangle_j \\
\langle 0|_i\langle 0|_j\ V\ |n2\rangle_i|m2\rangle_j & \langle 0|_i\langle 0|_j\ V\ |n2\rangle_i|0\rangle_j & \langle 0|_i\langle 0|_j\ V\ |0\rangle_i|m2\rangle_j & \langle 0|_i\langle 0|_j\ V\ |0\rangle_i|0\rangle_j
\end{pmatrix}$$

Deal with Kronecker delta and summation (no easy way to do it)

In[337]:=
```
Sum[x_{i,j} * DiscreteDelta[i - j], {i, 1, Infinity}]
```

Out[337]= $x_{j,j}$ UnitStep[-1 + j]

In[338]:=
```
Simplify[x_{j,j} UnitStep[-1 + j], j ≥ 1]
```

Out[338]= $x_{j,j}$

In[339]:=
```
Sum[x_{i,j} * DiscreteDelta[i - M] DiscreteDelta[j - L], {i, 1, Infinity}, {j, 1, Infinity}]
```

Out[339]= $x_{M,L}$ UnitStep[-1 + L] UnitStep[-1 + M]

We have to do it in a cumbersome way

In[340]:=
```
A1 = Sum[Sum[dd[G, G, V_{k,j}, G, M], {k, 1, nmol}], {M, 1, nrot}]
A2 = Sum[Sum[dd[G, M, V_{k,j}, G, G], {k, 1, nmol}], {M, 1, nrot}]
B1 = 1/2 Sum[dd[G, G, V_{i,j}, M, L], {M, 1, nrot}, {L, 1, nrot}]
B2 = 1/2 Sum[dd[M, L, V_{i,j}, G, G], {M, 1, nrot}, {L, 1, nrot}]
B3 = Sum[dd[G, L, V_{i,j}, M, G], {M, 1, nrot}, {L, 1, nrot}]
B4 = Sum[Sum[(1 - δ_{L, M}) * dd[L, G, V_{i,k}, M, G], {k, 1, nmol}], {M, 1, nrot}, {L, 1, nrot}]
B5 = Sum[(ε_M - ε_0) + Sum[dd[M, G, V_{i,k}, M, G] - dd[G, G, V_{i,k}, G, G], {k, 1, nmol}], {M, 1, nrot}]

C1 = Sum[dd[M, G, V_{i,j}, M2, L] - δ_{M, M2} dd[G, G, V_{i,j}, G, L],
   {M, 1, nrot}, {M2, 1, nrot}, {L, 1, nrot}] (* M2 represents M' *)
C2 = Sum[dd[M, L, V_{i,j}, M2, G] - δ_{M, M2} dd[G, L, V_{i,j}, G, G],
   {M, 1, nrot}, {M2, 1, nrot}, {L, 1, nrot}]
D1 = 1/2 Sum[δ_{M, M2} δ_{L, L2} dd[G, G, V_{i,j}, G, G] - 2 δ_{L, L2} dd[M, G, V_{i,j}, M2, G] + dd[M, L, V_{i,j}, M2, L2],
    {M, 1, nrot}, {M2, 1, nrot}, {L, 1, nrot}, {L2, 1, nrot}]

coefficients = {
    A1,
    A2,
    B1,
    B2,
    B3,
    B4,
    B5,
    C1,
    C2,
    D1
   };
```

Out[340]= $$\sum_{M=1}^{nrot}\left(\sum_{k=1}^{nmol} dd[G, G, V_{k,j}, G, M]\right)$$

Out[341]= $$\sum_{M=1}^{nrot}\left(\sum_{k=1}^{nmol} dd[G, M, V_{k,j}, G, G]\right)$$

Out[342]= $$\frac{1}{2}\sum_{M=1}^{nrot}\sum_{L=1}^{nrot} dd[G, G, V_{i,j}, M, L]$$

Out[343]= $$\frac{1}{2}\sum_{M=1}^{nrot}\sum_{L=1}^{nrot} dd[M, L, V_{i,j}, G, G]$$

Out[344]= $$\sum_{M=1}^{nrot}\sum_{L=1}^{nrot} dd[G, L, V_{i,j}, M, G]$$

Out[345]= $$\sum_{M=1}^{nrot}\sum_{L=1}^{nrot}\left(\sum_{k=1}^{nmol} dd[L, G, V_{i,k}, M, G]\,(1-\delta_{L,M})\right)$$

Out[346]= $$\sum_{M=1}^{nrot}\left(-\varepsilon_0+\varepsilon_M+\sum_{k=1}^{nmol}(-dd[G, G, V_{i,k}, G, G]+dd[M, G, V_{i,k}, M, G])\right)$$

Out[347]= $$\sum_{M=1}^{nrot}\sum_{M2=1}^{nrot}\sum_{L=1}^{nrot}\left(dd[M, G, V_{i,j}, M2, L]-dd[G, G, V_{i,j}, G, L]\,\delta_{M,M2}\right)$$

Out[348]= $$\sum_{M=1}^{nrot}\sum_{M2=1}^{nrot}\sum_{L=1}^{nrot}\left(dd[M, L, V_{i,j}, M2, G]-dd[G, L, V_{i,j}, G, G]\,\delta_{M,M2}\right)$$

Out[349]= $$\frac{1}{2}\sum_{M=1}^{nrot}\sum_{M2=1}^{nrot}\sum_{L=1}^{nrot}\sum_{L2=1}^{nrot}\left(dd[M, L, V_{i,j}, M2, L2]-2\,dd[M, G, V_{i,j}, M2, G]\,\delta_{L,L2}+dd[G, G, V_{i,j}, G, G]\,\delta_{L,L2}\,\delta_{M,M2}\right)$$

In[351]:=
```
ham2 = ham;
Do[
 Print[
  "*********************************************************************************"];
 ham2⟦i1, j1⟧ = coefficients.ham⟦i1, j1⟧;
 Print[braketmat⟦i1, j1⟧, " = ", ham2⟦i1, j1⟧];
 Print[" "];
 Print[" "],
 {i1, 1, Length[lolist]},
 {j1, 1, Length[lolist]}
]
```

```
*********************************************************************************
```

$$\langle n1|_i\langle m1|_j\ V\ |n2\rangle_i|m2\rangle_j =$$

$$(\delta_{M,n2}\,\delta_{m1,m2}\,\delta_{n1,M}+\delta_{M,m2}\,\delta_{m1,M}\,\delta_{n1,n2})\sum_{M=1}^{nrot}\left(-\varepsilon_0+\varepsilon_M+\sum_{k=1}^{nmol}(-dd[G, G, V_{i,k}, G, G]+dd[M, G, V_{i,k}, M, G])\right)+$$

$$(\delta_{M,n2}\,\delta_{m1,m2}\,\delta_{n1,L}+\delta_{M,m2}\,\delta_{m1,L}\,\delta_{n1,n2})\sum_{M=1}^{nrot}\sum_{L=1}^{nrot}\left(\sum_{k=1}^{nmol} dd[L, G, V_{i,k}, M, G]\,(1-\delta_{L,M})\right)+$$

$$\frac{1}{2}(\delta_{L2,n2}\,\delta_{m1,M}\,\delta_{M2,m2}\,\delta_{n1,L}+\delta_{L2,m2}\,\delta_{m1,L}\,\delta_{M2,n2}\,\delta_{n1,M})$$

$$\sum_{M=1}^{nrot}\sum_{M2=1}^{nrot}\sum_{L=1}^{nrot}\sum_{L2=1}^{nrot}\left(dd[M, L, V_{i,j}, M2, L2]-2\,dd[M, G, V_{i,j}, M2, G]\,\delta_{L,L2}+dd[G, G, V_{i,j}, G, G]\,\delta_{L,L2}\,\delta_{M,M2}\right)$$

```
*********************************************************************************
```

$$\langle n1|_i \langle m1|_j\ V\ |n2\rangle_i |0\rangle_j = \delta_{m1,M}\,\delta_{n1,n2} \sum_{M=1}^{nrot} \left(\sum_{k=1}^{nmol} dd[G, M, V_{k,j}, G, G] \right) + \delta_{m1,L}\,\delta_{M2,n2}\,\delta_{n1,M} \sum_{M=1}^{nrot} \sum_{M2=1}^{nrot} \sum_{L=1}^{nrot} \left(dd[M, L, V_{i,j}, M2, G] - dd[G, L, V_{i,j}, G, G]\,\delta_{M,M2} \right)$$

****

$$\langle n1|_i \langle m1|_j\ V\ |0\rangle_i |m2\rangle_j = \delta_{m1,m2}\,\delta_{n1,M} \sum_{M=1}^{nrot} \left(\sum_{k=1}^{nmol} dd[G, M, V_{k,j}, G, G] \right) + \delta_{m1,M}\,\delta_{M2,m2}\,\delta_{n1,L} \sum_{M=1}^{nrot} \sum_{M2=1}^{nrot} \sum_{L=1}^{nrot} \left(dd[M, L, V_{i,j}, M2, G] - dd[G, L, V_{i,j}, G, G]\,\delta_{M,M2} \right)$$

****

$$\langle n1|_i \langle m1|_j\ V\ |0\rangle_i |0\rangle_j = \frac{1}{2} (\delta_{m1,M}\,\delta_{n1,L} + \delta_{m1,L}\,\delta_{n1,M}) \sum_{M=1}^{nrot} \sum_{L=1}^{nrot} dd[M, L, V_{i,j}, G, G]$$

****

$$\langle n1|_i \langle 0|_j\ V\ |n2\rangle_i |m2\rangle_j = \delta_{M,m2}\,\delta_{n1,n2} \sum_{M=1}^{nrot} \left(\sum_{k=1}^{nmol} dd[G, G, V_{k,j}, G, M] \right) + \delta_{L,m2}\,\delta_{M2,n2}\,\delta_{n1,M} \sum_{M=1}^{nrot} \sum_{M2=1}^{nrot} \sum_{L=1}^{nrot} \left(dd[M, G, V_{i,j}, M2, L] - dd[G, G, V_{i,j}, G, L]\,\delta_{M,M2} \right)$$

****

$$\langle n1|_i \langle 0|_j\ V\ |n2\rangle_i |0\rangle_j = \delta_{M,n2}\,\delta_{n1,M} \sum_{M=1}^{nrot} \left(-\varepsilon_0 + \varepsilon_M + \sum_{k=1}^{nmol} (-dd[G, G, V_{i,k}, G, G] + dd[M, G, V_{i,k}, M, G]) \right) + \delta_{M,n2}\,\delta_{n1,L} \sum_{M=1}^{nrot} \sum_{L=1}^{nrot} \left(\sum_{k=1}^{nmol} dd[L, G, V_{i,k}, M, G]\,(1 - \delta_{L,M}) \right)$$

****

$$\langle n1|_i \langle 0|_j\ V\ |0\rangle_i |m2\rangle_j = \delta_{M,m2}\,\delta_{n1,L} \sum_{M=1}^{nrot} \sum_{L=1}^{nrot} dd[G, L, V_{i,j}, M, G]$$

****

$$\langle n1|_i \langle 0|_j \; V \; |0\rangle_i |0\rangle_j = \delta_{n1,M} \sum_{M=1}^{nrot} \left(\sum_{k=1}^{nmol} dd[G, M, V_{k,j}, G, G] \right)$$

****

$$\langle 0|_i \langle m1|_j \; V \; |n2\rangle_i |m2\rangle_j = \delta_{M,n2}\, \delta_{m1,m2} \sum_{M=1}^{nrot} \left(\sum_{k=1}^{nmol} dd[G, G, V_{k,j}, G, M] \right) + \delta_{L,n2}\, \delta_{m1,M}\, \delta_{M2,m2} \sum_{M=1}^{nrot} \sum_{M2=1}^{nrot} \sum_{L=1}^{nrot} \left(dd[M, G, V_{i,j}, M2, L] - dd[G, G, V_{i,j}, G, L]\, \delta_{M,M2} \right)$$

****

$$\langle 0|_i \langle m1|_j \; V \; |n2\rangle_i |0\rangle_j = \delta_{M,n2}\, \delta_{m1,L} \sum_{M=1}^{nrot} \sum_{L=1}^{nrot} dd[G, L, V_{i,j}, M, G]$$

****

$$\langle 0|_i \langle m1|_j \; V \; |0\rangle_i |m2\rangle_j = \delta_{M,m2}\, \delta_{m1,M} \sum_{M=1}^{nrot} \left(-\varepsilon_0 + \varepsilon_M + \sum_{k=1}^{nmol} \left(-dd[G, G, V_{i,k}, G, G] + dd[M, G, V_{i,k}, M, G] \right) \right) + \delta_{M,m2}\, \delta_{m1,L} \sum_{M=1}^{nrot} \sum_{L=1}^{nrot} \left(\sum_{k=1}^{nmol} dd[L, G, V_{i,k}, M, G]\, (1 - \delta_{L,M}) \right)$$

****

$$\langle 0|_i \langle m1|_j \; V \; |0\rangle_i |0\rangle_j = \delta_{m1,M} \sum_{M=1}^{nrot} \left(\sum_{k=1}^{nmol} dd[G, M, V_{k,j}, G, G] \right)$$

****

$$\langle 0|_i \langle 0|_j \; V \; |n2\rangle_i |m2\rangle_j = \frac{1}{2} (\delta_{L,n2}\, \delta_{M,m2} + \delta_{L,m2}\, \delta_{M,n2}) \sum_{M=1}^{nrot} \sum_{L=1}^{nrot} dd[G, G, V_{i,j}, M, L]$$

****

$$\langle 0|_i \langle 0|_j \; V \; |n2\rangle_i |0\rangle_j \; = \; \delta_{M,n2} \sum_{M=1}^{nrot} \left(\sum_{k=1}^{nmol} dd[G, G, V_{k,j}, G, M] \right)$$

****

$$\langle 0|_i \langle 0|_j \; V \; |0\rangle_i |m2\rangle_j \; = \; \delta_{M,m2} \sum_{M=1}^{nrot} \left(\sum_{k=1}^{nmol} dd[G, G, V_{k,j}, G, M] \right)$$

****

$$\langle 0|_i \langle 0|_j \; V \; |0\rangle_i |0\rangle_j \; = \; 0$$

Final results

$$\langle \mathrm{n1}\,|_i\ \langle \mathrm{m1}\,|_j\ H\ |\,\mathrm{n2}\rangle_i\ \big|\,\mathrm{m2}\big\rangle_j$$

$$= \delta_{\mathrm{m1,m2}}\,\delta_{\mathrm{n1,n2}}\Big\{(\varepsilon_{\mathrm{n1}} - \varepsilon_0) + \sum_{k=1}^{\mathrm{nmol}}\Big[\big\langle \mathrm{n1},\, G\,\big|\, V_{i,k}\,\big|\,\mathrm{n1},\, G\big\rangle - \big\langle G,\, G\,\big|\,V_{i,k}\,\big|\,G,\,G\big\rangle\Big] +$$

$$(\varepsilon_{\mathrm{m1}} - \varepsilon_0) + \sum_{k=1}^{\mathrm{nmol}}\Big[\big\langle \mathrm{m1},\, G\,\big|\, V_{j,k}\,\big|\,\mathrm{m1},\, G\big\rangle - \big\langle G,\, G\,\big|\,V_{j,k}\,\big|\,G,\,G\big\rangle\Big]\Big\}$$

$$+\ \delta_{\mathrm{m1,m2}}\sum_{k=1}^{\mathrm{nmol}}\Big[\big\langle \mathrm{n1},\, G\,\big|\,V_{i,k}\,\big|\,\mathrm{n2},\,G\big\rangle\big(1 - \delta_{\mathrm{n1,\,n2}}\big)\Big] +$$

$$\delta_{\mathrm{n1,n2}}\sum_{k=1}^{\mathrm{nmol}}\Big[\big\langle \mathrm{m1},\, G\,\big|\,V_{j,k}\,\big|\,\mathrm{m2},\,G\big\rangle\big(1 - \delta_{\mathrm{m1,\,m2}}\big)\Big]$$

$$+\ \frac{1}{2}\Big[\ \langle \mathrm{m1},\, \mathrm{n1}\,|\,V_{i,j}\,|\,\mathrm{m2},\,\mathrm{n2}\rangle -$$

$$2\,\langle \mathrm{m1},\,G\,|\,V_{i,j}\,|\,\mathrm{m2},\,G\rangle\,\delta_{\mathrm{n1,n2}} + \langle G,\,G\,|\,V_{i,j}\,|\,G,\,G\rangle\,\delta_{\mathrm{n1,\,n2}}\,\delta_{\mathrm{m1,\,m2}} +$$

$$\langle \mathrm{n1},\, \mathrm{m1}\,|\,V_{i,j}\,|\,\mathrm{n2},\,\mathrm{m2}\rangle -$$

$$2\,\langle \mathrm{n1},\,G\,|\,V_{i,j}\,|\,\mathrm{n2},\,G\rangle\,\delta_{\mathrm{m1,\,m2}} + \langle G,\,G\,|\,V_{i,j}\,|\,G,\,G\rangle\,\delta_{\mathrm{m1,\,m2}}\,\delta_{\mathrm{n1,\,n2}}\Big]$$

In[353]:=

$$\langle \mathrm{n1}\,|_i\ \langle \mathrm{m1}\,|_j\ H\ |\,\mathrm{n2}\rangle_i\ \big|\,0\big\rangle_j$$

$$= \delta_{\mathrm{n1,n2}}\sum_{k=1}^{\mathrm{nmol}}\big\langle G,\,\mathrm{m1}\,\big|\,V_{k,j}\,\big|\,G,\,G\big\rangle$$

$$+\ \langle \mathrm{n1},\,\mathrm{m1}\,|\,V_{i,j}\,|\,\mathrm{n2},\,G\rangle - \langle G,\,\mathrm{m1}\,|\,V_{i,j}\,|\,G,\,G\rangle\,\delta_{\mathrm{n1,\,n2}}$$

In[354]:=

$$\langle \text{n1} |_i \ \langle \text{m1} |_j \, H \, | \, 0\rangle_i \, \big| \, \text{m2}\big\rangle_j = \delta_{\text{m1, m2}} \sum_{k=1}^{\text{nmol}} \big\langle G, \text{n1} \, | \, V_{k,i} \, | \, G, G\big\rangle$$
$$+ \langle \text{m1, n1} \, | \, V_{i,j} \, | \, \text{m2}, G\rangle - \langle G, \text{n1} \, | \, V_{i,j} \, | \, G, G\rangle \, \delta_{\text{m1, m2}}$$

In[355]:=

$$\langle \text{n1} |_i \ \langle \text{m1} |_j \, H \, | \, 0\rangle_i \, \big| \, 0\big\rangle_j = \frac{1}{2} \left[\langle \text{m1, n1} \, | \, V_{i,j} \, | \, G, G\rangle + \langle \text{n1, m1} \, | \, V_{i,j} \, | \, G, G\rangle\right]$$

In[356]:=

$$\langle \text{n1} |_i \ \langle 0 |_j \, H \, | \, \text{n2}\rangle_i \, \big| \, \text{m2}\big\rangle_j = \delta_{\text{n1,n2}} \sum_{k=1}^{\text{nmol}} \big\langle G, G \, | \, V_{k,j} \, | \, G, \text{m2}\big\rangle +$$
$$\langle \text{n1}, G \, | \, V_{i,j} \, | \, \text{n2, m2}\rangle - \langle G, G \, | \, V_{i,j} \, | \, G, \text{m2}\rangle \, \delta_{\text{n1, n2}}$$

In[357]:=

$$\langle \text{n1} |_i \ \langle 0 |_j \, H \, | \, \text{n2}\rangle_i \, \big| \, 0\big\rangle_j =$$
$$\delta_{\text{n1, n2}} \left(-\varepsilon_0 + \varepsilon_{\text{n1}} + \sum_{k=1}^{\text{nmol}} \left[\big\langle \text{n1}, G \, | \, V_{i,k} \, | \, \text{n1}, G\big\rangle - \big\langle G, G \, | \, V_{i,k} \, | \, G, G\big\rangle\right]\right)$$
$$+ \sum_{k=1}^{\text{nmol}} \big\langle \text{n1}, G \, | \, V_{i,k} \, | \, \text{n2}, G\big\rangle \left(1 - \delta_{\text{n1, n2}}\right)$$

In[358]:=

$$\langle \text{n1} |_i \ \langle 0 |_j \, H \, | \, 0\rangle_i \, \big| \, \text{m2}\big\rangle_j = \langle G, \text{n1} \, | \, V_{i,j} \, | \, \text{m2}, G\rangle$$

In[359]:=

$$\langle \text{n1} |_i \ \langle 0 |_j \, H \, | \, 0\rangle_i \, \big| \, 0\big\rangle_j = \sum_{k=1}^{\text{nmol}} \big\langle G, \text{n1} \, | \, V_{k,i} \, | \, G, G\big\rangle$$

In[360]:=

$$\langle 0 |_i \ \langle \text{m1} |_j \, H \, | \, \text{n2}\rangle_i \, \big| \, \text{m2}\big\rangle_j = \delta_{\text{m1,m2}} \sum_{k=1}^{\text{nmol}} \big\langle G, G \, | \, V_{k,i} \, | \, G, \text{n2}\big\rangle +$$
$$\langle \text{m1}, G \, | \, V_{i,j} \, | \, \text{m2, n2}\rangle - \langle G, G \, | \, V_{i,j} \, | \, G, \text{n2}\rangle \, \delta_{\text{m1, m2}}$$

$$\langle 0 |_i \ \langle \text{m1} |_j\, H \,|\, \text{n2}\rangle_i \,\big|\, 0\big\rangle_j = \langle G,\, \text{m1} \,|\, V_{i,j} \,|\, \text{n2},\ G\rangle$$

$$\langle 0 |_i \ \langle \text{m1} |_j\, H \,|\, 0\rangle_i \,\big|\, \text{m2}\big\rangle_j = \delta_{\text{m1},\text{m2}}$$

$$\left\{(\varepsilon_{\text{m1}} - \varepsilon_0) + \sum_{k=1}^{\text{nmol}} \left[\left\langle \text{m1},\, G \,|\, V_{j,\,k} \,|\, \text{m1},\, G\right\rangle - \left\langle G,\, G \,|\, V_{j,\,k} \,|\, G,\, G\right\rangle\right]\right\}$$

$$+ \sum_{k=1}^{\text{nmol}} \left\langle \text{m1},\, G \,|\, V_{j,\,k} \,|\, \text{m2},\, G\right\rangle \left(1 - \delta_{\text{m1},\text{m2}}\right)$$

$$\langle 0 |_i \ \langle \text{m1} |_j\, H \,|\, 0\rangle_i \,\big|\, 0\big\rangle_j = \sum_{k=1}^{\text{nmol}} \left\langle G,\ \text{m1} \,|\, V_{k,\,j} \,|\, G,\, G\right\rangle$$

$$\langle 0 |_i \ \langle 0 |_j\, H \,|\, \text{n2}\rangle_i \,\big|\, \text{m2}\big\rangle_j = \frac{1}{2}\left[\langle G,\, G \,|\, V_{i,j} \,|\, \text{m2},\, \text{n2}\rangle + \langle G,\, G \,|\, V_{i,\,j} \,|\, \text{n2},\, \text{m2}\rangle\right]$$

$$\langle 0 |_i \ \langle 0 |_j\, H \,|\, \text{n2}\rangle_i \,\big|\, 0\big\rangle_j = \sum_{k=1}^{\text{nmol}} \left\langle G,\, G \,|\, V_{k,\,i} \,|\, G,\, \text{n2}\right\rangle$$

$$\langle 0 |_i \ \langle 0 |_j\, H \,|\, 0\rangle_i \,\big|\, \text{m2}\big\rangle_j = \sum_{k=1}^{\text{nmol}} \left\langle G,\, G \,|\, V_{k,\,j} \,|\, G,\, \text{m2}\right\rangle$$

$$\langle 0 |_i \ \langle 0 |_j\, H \,|\, 0\rangle_i \,\big|\, 0\big\rangle_j = 0$$