Exact Hamiltonian for multi-level system

Substitutions that needed in the derivations

$\left(P^{\dagger}\right)_{n,M} = \left(b^{\dagger}\right)_{n,M} b_{n,G}$ and $P_{n,M} = \left(b^{\dagger}\right)_{n,G} b_{n,M}$ and $\left(b^{\dagger}\right)_{n,M} b_{n,K} = \left(P^{\dagger}\right)_{n,M} P_{n,K}$

```
Clear["Global`*"]
sub1 = (b†)_{n_,M_} ** b_{n_,G} /; UnsameQ[M, G] :> (P†)_{n,M};
(*sub2 = b_{n_,G} ** (b†)_{n_,M_} /;UnsameQ[M,G]:>(P†)_{n,M}; *)
sub3 = (b†)_{n_,G} ** b_{n_,M_} /; UnsameQ[M, G] :> P_{n,M};
(*sub4= b_{n_,M_} ** (b†)_{n_,G} /;UnsameQ[M,G]:> P_{n,M};*)
sub5 = (b†)_{n_,M_} ** b_{n_,K_} /; UnsameQ[M, G] && UnsameQ[K, G] :> (P†)_{n,M} ** P_{n,K};
```

```
(* G represents the gound state, M1, L1, M2, L2 represent any excited states *)
term1 = Apply[
  Plus, Flatten[Outer[f, {G, M1}, {G, L1}, {G, M2}, {G, L2}]]
 ]
```

```
f[G, G, G, G] + f[G, G, G, L2] + f[G, G, M2, G] + f[G, G, M2, L2] + f[G, L1, G, G] + f[G, L1, G, L2] +
 f[G, L1, M2, G] + f[G, L1, M2, L2] + f[M1, G, G, G] + f[M1, G, G, L2] + f[M1, G, M2, G] +
 f[M1, G, M2, L2] + f[M1, L1, G, G] + f[M1, L1, G, L2] + f[M1, L1, M2, G] + f[M1, L1, M2, L2]
```

```
(* Combine terms that are equivalent ( by exchanging molecule index n and m) *)
sublist = {
   (* 3 G in the square bracket *)
   f[G, G, m_, G] /; m =!= G → f[G, G, G, L2],
   f[G, G, G, m_] /; m =!= G → f[G, G, G, L2],

   f[G, m_, G, G] /; m =!= G → f[G, L1, G, G],
   f[m_, G, G, G] /; m =!= G → f[G, L1, G, G],

   (* 2 G in the square bracket *)
   f[G, m_, n_, G] /; m =!= G && n =!= G → f[G, L1, M2, G],
   f[m_, G, G, n_] /; m =!= G && n =!= G → f[G, L1, M2, G],

   f[G, m_, G, n_] /; m =!= G && n =!= G → f[M1, G, M2, G],
   f[m_, G, n_, G] /; m =!= G && n =!= G → f[M1, G, M2, G],

   (* 1 G in the square bracket *)
   f[G, p_, m_, n_] /; m =!= G && n =!= G && p =!= G → f[G, L1, M2, L2],
   f[p_, G, m_, n_] /; m =!= G && n =!= G && p =!= G → f[G, L1, M2, L2], (* the order of
    index L1, M2 doesn't matter because one order just corresponds to one renaming *)

   f[p_, m_, n_, G] /; m =!= G && n =!= G && p =!= G → f[M1, L1, M2, G],
   f[p_, m_, G, n_] /; m =!= G && n =!= G && p =!= G → f[M1, L1, M2, G]
  };
term2 = term1 /. sublist
```

```
f[G, G, G, G] + 2 f[G, G, G, L2] + f[G, G, M2, L2] + 2 f[G, L1, G, G] + 2 f[G, L1, M2, G] +
 2 f[G, L1, M2, L2] + 2 f[M1, G, M2, G] + f[M1, L1, G, G] + 2 f[M1, L1, M2, G] + f[M1, L1, M2, L2]
```

```
(* adding the operator corresponding to each f *)
(* Note f[M1,L1,M2,L2]=<M1|_{n} <L1|_m |V |M2>_{n} |L2>_{m} *)
(* M1, M2 are states for molecule i, L1, L2 are states for molecule j *)
f[M1_, L1_, M2_, L2_] := mat[M1, L1, M2, L2] (b†)_{i,M1} ** b_{i,M2} ** (b†)_{j,L1} ** b_{j,L2}
term3 = term2 //. {sub1, sub3, sub5}
```

$\text{mat}[G, G, M2, L2]\, P_{i,M2} ** P_{j,L2} + 2\,\text{mat}[G, L1, M2, G]\, P_{i,M2} ** (P^\dagger)_{j,L1} +$
$\text{mat}[M1, L1, G, G]\, (P^\dagger)_{i,M1} ** (P^\dagger)_{j,L1} + 2\,\text{mat}[G, L1, M2, L2]\, P_{i,M2} ** (P^\dagger)_{j,L1} ** P_{j,L2} +$
$2\,\text{mat}[G, G, G, L2]\, (b^\dagger)_{i,G} ** b_{i,G} ** P_{j,L2} + 2\,\text{mat}[G, L1, G, G]\, (b^\dagger)_{i,G} ** b_{i,G} ** (P^\dagger)_{j,L1} +$
$2\,\text{mat}[M1, L1, M2, G]\, (P^\dagger)_{i,M1} ** P_{i,M2} ** (P^\dagger)_{j,L1} + \text{mat}[G, G, G, G]\, (b^\dagger)_{i,G} ** b_{i,G} ** (b^\dagger)_{j,G} ** b_{j,G} +$
$2\,\text{mat}[M1, G, M2, G]\, (P^\dagger)_{i,M1} ** P_{i,M2} ** (b^\dagger)_{j,G} ** b_{j,G} +$
$\text{mat}[M1, L1, M2, L2]\, (P^\dagger)_{i,M1} ** P_{i,M2} ** (P^\dagger)_{j,L1} ** P_{j,L2}$

```
(* get rid of (b†)_{j,G}**b_{j,G} terms *)
sub6 = {(b†)_{n_,G} ** b_{n_,G} ** (b†)_{m_,G} ** b_{m_,G} :> (1 - 2 (P†)_{n,R} ** P_{n,R} + (P†)_{n,S} ** P_{n,S} ** (P†)_{m,R} ** P_{m,R}),
    (b†)_{n_,G} ** b_{n_,G} :> 1 - (P†)_{n,R} ** P_{n,R}};
  (* Every index that is not G represent a summation *)
(* (P†)_{n,R}**P_{n,R} is actually a summation over state R (R ≠ G)*)
term4 = term3 /. sub6
```

$2\,\text{mat}[G, G, G, L2]\, (1 - (P^\dagger)_{i,R} ** P_{i,R}) ** P_{j,L2} + 2\,\text{mat}[G, L1, G, G]\, (1 - (P^\dagger)_{i,R} ** P_{i,R}) ** (P^\dagger)_{j,L1} +$
$\text{mat}[G, G, M2, L2]\, P_{i,M2} ** P_{j,L2} + 2\,\text{mat}[G, L1, M2, G]\, P_{i,M2} ** (P^\dagger)_{j,L1} +$
$\text{mat}[M1, L1, G, G]\, (P^\dagger)_{i,M1} ** (P^\dagger)_{j,L1} + 2\,\text{mat}[G, L1, M2, L2]\, P_{i,M2} ** (P^\dagger)_{j,L1} ** P_{j,L2} +$
$2\,\text{mat}[M1, G, M2, G]\, (P^\dagger)_{i,M1} ** P_{i,M2} ** (1 - (P^\dagger)_{j,R} ** P_{j,R}) +$
$2\,\text{mat}[M1, L1, M2, G]\, (P^\dagger)_{i,M1} ** P_{i,M2} ** (P^\dagger)_{j,L1} +$
$\text{mat}[M1, L1, M2, L2]\, (P^\dagger)_{i,M1} ** P_{i,M2} ** (P^\dagger)_{j,L1} ** P_{j,L2} +$
$\text{mat}[G, G, G, G]\, (1 - 2\,(P^\dagger)_{i,R} ** P_{i,R} + (P^\dagger)_{i,S} ** P_{i,S} ** (P^\dagger)_{j,R} ** P_{j,R})$

```
(* Expand the NonCommutativeMultiply products *)
ExpandNCM[(h : NonCommutativeMultiply)[a___, b_Plus, c___]] :=
 Distribute[h[a, b, c], Plus, h, Plus, ExpandNCM[h[##]] &]

ExpandNCM[(h : NonCommutativeMultiply)[a___, b_Times, c___]] :=
 Most[b] ExpandNCM[h[a, Last[b], c]]

ExpandNCM[a_] := ExpandAll[a]
(* to understand the above, see the following *)
(* Distribute[expr,g,f,gp,fp] gives gp and fp in place of g and f
 respectively in the result of the distribution. Distribute[exp, g, f]
 distribute over g only if the head of expr is f *)
(*INPUT:Distribute[(a+b+c)(u+v),Plus,Times,plus,times]
OUTPUT:plus[times[a,u],times[a,v],times[b,u],times[b,v],times[c,u],times[c,v]]
INPUT: Distribute[(a**b+c**d)**u,Plus,
       NonCommutativeMultiply,Plus,NonCommutativeMultiply[##]&]
OUTPUT: a**b**u+c**d**u*)
expand =
 Times[x___, NonCommutativeMultiply[h__], y___ ] :> x y ExpandNCM[NonCommutativeMultiply[h]]
```

NonCommutativeMultiply[h__] x___ y___ :> x y ExpandNCM[NonCommutativeMultiply[h]]

```
(* expand over the noncommutative multiplication *)
term5 = term4 /. expand
```

$$\begin{aligned}&\mathrm{mat}[G, G, M2, L2]\, P_{i,M2} ** P_{j,L2} + 2\,\mathrm{mat}[G, L1, M2, G]\, P_{i,M2} ** (P^\dagger)_{j,L1} +\\
&\mathrm{mat}[M1, L1, G, G]\, (P^\dagger)_{i,M1} ** (P^\dagger)_{j,L1} + 2\,\mathrm{mat}[G, L1, M2, L2]\, P_{i,M2} ** (P^\dagger)_{j,L1} ** P_{j,L2} +\\
&2\,\mathrm{mat}[M1, L1, M2, G]\, (P^\dagger)_{i,M1} ** P_{i,M2} ** (P^\dagger)_{j,L1} +\\
&2\,\mathrm{mat}[G, G, G, L2]\, \left(1 ** P_{j,L2} - (P^\dagger)_{i,R} ** P_{i,R} ** P_{j,L2}\right) +\\
&2\,\mathrm{mat}[G, L1, G, G]\, \left(1 ** (P^\dagger)_{j,L1} - (P^\dagger)_{i,R} ** P_{i,R} ** (P^\dagger)_{j,L1}\right) +\\
&\mathrm{mat}[M1, L1, M2, L2]\, (P^\dagger)_{i,M1} ** P_{i,M2} ** (P^\dagger)_{j,L1} ** P_{j,L2} +\\
&2\,\mathrm{mat}[M1, G, M2, G]\, \left((P^\dagger)_{i,M1} ** P_{i,M2} ** 1 - (P^\dagger)_{i,M1} ** P_{i,M2} ** (P^\dagger)_{j,R} ** P_{j,R}\right) +\\
&\mathrm{mat}[G, G, G, G]\, \left(1 - 2\,(P^\dagger)_{i,R} ** P_{i,R} + (P^\dagger)_{i,S} ** P_{i,S} ** (P^\dagger)_{j,R} ** P_{j,R}\right)\end{aligned}$$

```
(*get rid of extra 1*)
term8 = (term5 /. {1 ** x_ :> x, y_ ** 1 :> y, u_ ** 1 ** v_ :> u ** v}) // ExpandAll
```

$$\begin{aligned}&\mathrm{mat}[G, G, G, G] + \mathrm{mat}[G, G, M2, L2]\, P_{i,M2} ** P_{j,L2} + 2\,\mathrm{mat}[G, L1, M2, G]\, P_{i,M2} ** (P^\dagger)_{j,L1} +\\
&2\,\mathrm{mat}[M1, G, M2, G]\, (P^\dagger)_{i,M1} ** P_{i,M2} + \mathrm{mat}[M1, L1, G, G]\, (P^\dagger)_{i,M1} ** (P^\dagger)_{j,L1} -\\
&2\,\mathrm{mat}[G, G, G, G]\, (P^\dagger)_{i,R} ** P_{i,R} + 2\,\mathrm{mat}[G, L1, M2, L2]\, P_{i,M2} ** (P^\dagger)_{j,L1} ** P_{j,L2} +\\
&2\,\mathrm{mat}[M1, L1, M2, G]\, (P^\dagger)_{i,M1} ** P_{i,M2} ** (P^\dagger)_{j,L1} - 2\,\mathrm{mat}[G, G, G, L2]\, (P^\dagger)_{i,R} ** P_{i,R} ** P_{j,L2} -\\
&2\,\mathrm{mat}[G, L1, G, G]\, (P^\dagger)_{i,R} ** P_{i,R} ** (P^\dagger)_{j,L1} + \mathrm{mat}[M1, L1, M2, L2]\, (P^\dagger)_{i,M1} ** P_{i,M2} ** (P^\dagger)_{j,L1} ** P_{j,L2} -\\
&2\,\mathrm{mat}[M1, G, M2, G]\, (P^\dagger)_{i,M1} ** P_{i,M2} ** (P^\dagger)_{j,R} ** P_{j,R} +\\
&\mathrm{mat}[G, G, G, G]\, (P^\dagger)_{i,S} ** P_{i,S} ** (P^\dagger)_{j,R} ** P_{j,R} + 2\,\mathrm{mat}[G, G, G, L2]\, P_{j,L2} + 2\,\mathrm{mat}[G, L1, G, G]\, (P^\dagger)_{j,L1}\end{aligned}$$

```
(* expand the bracket *)
(*term6=ExpandAll[term5]*)
```

```
(* get rid of 1 *)
(*term7=term6/. NonCommutativeMultiply[x___,1,y___]→ NonCommutativeMultiply[x,y]*)
```

```
(* get rid of NonCommutativeMultiply with a single variable *)
(*term8=term7/.NonCommutativeMultiply[x_]→ x*)
```

```
(* whenever I write M, it means the summation of M *)
(* every index M, M1, M2, L1, L2, R means summation *)
(* term0 comes from H_rot and the abover term8 comes from V_dd *)
```

$$\text{term0} = \varepsilon_0 \left(b^\dagger\right)_{i,G} ** b_{i,G} + \varepsilon_M \left(b^\dagger\right)_{i,M} ** b_{i,M} \;/.\; \left\{\left(b^\dagger\right)_{i,G} ** b_{i,G} \to 1 - \left(b^\dagger\right)_{i,M} ** b_{i,M}\right\}$$

```
term0 = Expand[term0]
(* collect the terms with the same operators *)
collect1 = Times[x_, NonCommutativeMultiply[h_]] + Times[y_, NonCommutativeMultiply[h_]] :→
   (x + y) NonCommutativeMultiply[h];
term0 = term0 /. collect1
term0 = term0 /. sub5
```

$$\left(1 - \left(b^\dagger\right)_{i,M} ** b_{i,M}\right) \varepsilon_0 + \left(b^\dagger\right)_{i,M} ** b_{i,M}\, \varepsilon_M$$

$$\varepsilon_0 - \left(b^\dagger\right)_{i,M} ** b_{i,M}\, \varepsilon_0 + \left(b^\dagger\right)_{i,M} ** b_{i,M}\, \varepsilon_M$$

$$\varepsilon_0 + \left(b^\dagger\right)_{i,M} ** b_{i,M} \left(-\varepsilon_0 + \varepsilon_M\right)$$

$$\varepsilon_0 + \left(P^\dagger\right)_{i,M} ** P_{i,M} \left(-\varepsilon_0 + \varepsilon_M\right)$$

$$\text{term9} = \text{Distribute}\left[\frac{1}{2}\,\text{term8}\right] + \text{term0}$$

$$\frac{1}{2}\,\text{mat}[G, G, G, G] + \frac{1}{2}\,\text{mat}[G, G, M2, L2]\, P_{i,M2} ** P_{j,L2} + \text{mat}[G, L1, M2, G]\, P_{i,M2} ** \left(P^\dagger\right)_{j,L1} +$$
$$\text{mat}[M1, G, M2, G] \left(P^\dagger\right)_{i,M1} ** P_{i,M2} + \frac{1}{2}\,\text{mat}[M1, L1, G, G] \left(P^\dagger\right)_{i,M1} ** \left(P^\dagger\right)_{j,L1} -$$
$$\text{mat}[G, G, G, G] \left(P^\dagger\right)_{i,R} ** P_{i,R} + \text{mat}[G, L1, M2, L2]\, P_{i,M2} ** \left(P^\dagger\right)_{j,L1} ** P_{j,L2} +$$
$$\text{mat}[M1, L1, M2, G] \left(P^\dagger\right)_{i,M1} ** P_{i,M2} ** \left(P^\dagger\right)_{j,L1} - \text{mat}[G, G, G, L2] \left(P^\dagger\right)_{i,R} ** P_{i,R} ** P_{j,L2} -$$
$$\text{mat}[G, L1, G, G] \left(P^\dagger\right)_{i,R} ** P_{i,R} ** \left(P^\dagger\right)_{j,L1} + \frac{1}{2}\,\text{mat}[M1, L1, M2, L2] \left(P^\dagger\right)_{i,M1} ** P_{i,M2} ** \left(P^\dagger\right)_{j,L1} ** P_{j,L2} -$$
$$\text{mat}[M1, G, M2, G] \left(P^\dagger\right)_{i,M1} ** P_{i,M2} ** \left(P^\dagger\right)_{j,R} ** P_{j,R} + \frac{1}{2}\,\text{mat}[G, G, G, G] \left(P^\dagger\right)_{i,S} ** P_{i,S} ** \left(P^\dagger\right)_{j,R} ** P_{j,R} +$$
$$\varepsilon_0 + \left(P^\dagger\right)_{i,M} ** P_{i,M} \left(-\varepsilon_0 + \varepsilon_M\right) + \text{mat}[G, G, G, L2]\, P_{j,L2} + \text{mat}[G, L1, G, G] \left(P^\dagger\right)_{j,L1}$$

```
(* find patterns and regroup terms *)
find[term_, pattern_] := Apply[Plus, Cases[Apply[List, term], pattern]]
(* include zero or one operator *)
p1 = Except[ Times[___, NonCommutativeMultiply[___]]];

(* include two operator *)

(* Pdiag**Pdiag and P**P *)
p2 = Alternatives[
   Times[___, NonCommutativeMultiply[(P†)__, (P†)__]],
   Times[___, NonCommutativeMultiply[P__, P__] ]
  ];
(* P**Pdiag and Pdiag**P *)
p3 = Alternatives[
   Times[___, NonCommutativeMultiply[P__, (P†)__] ],
   Times[___, NonCommutativeMultiply[(P†)__, P__] ]
  ];

(* three operators *)
p4 = Times[___, NonCommutativeMultiply[P__ | (P†)__, P__ | (P†)__, P__ | (P†)__] ];
Print["part 1"]
part1 = find[term9, p1]
Print["part 2"]
part2 = find[term9, p2]
Print["part 3"]
part3 = find[term9, p3]
Print["part 4"]
part4 = find[term9, p4]
Print["part 5"] (* terms with 4 operators *)
part5 = term9 - (part1 + part2 + part3 + part4)
```

part 1

$$\frac{1}{2}\,\mathrm{mat}[G, G, G, G] + \varepsilon_0 + \mathrm{mat}[G, G, G, L2]\,P_{j,L2} + \mathrm{mat}[G, L1, G, G]\,\left(P^\dagger\right)_{j,L1}$$

part 2

$$\frac{1}{2}\,\mathrm{mat}[G, G, M2, L2]\,P_{i,M2} ** P_{j,L2} + \frac{1}{2}\,\mathrm{mat}[M1, L1, G, G]\,\left(P^\dagger\right)_{i,M1} ** \left(P^\dagger\right)_{j,L1}$$

part 3

$$\mathrm{mat}[G, L1, M2, G]\,P_{i,M2} ** \left(P^\dagger\right)_{j,L1} + \mathrm{mat}[M1, G, M2, G]\,\left(P^\dagger\right)_{i,M1} ** P_{i,M2} - \mathrm{mat}[G, G, G, G]\,\left(P^\dagger\right)_{i,R} ** P_{i,R} + \left(P^\dagger\right)_{i,M} ** P_{i,M}\,(-\varepsilon_0 + \varepsilon_M)$$

part 4

$$\mathrm{mat}[G, L1, M2, L2]\,P_{i,M2} ** \left(P^\dagger\right)_{j,L1} ** P_{j,L2} + \mathrm{mat}[M1, L1, M2, G]\,\left(P^\dagger\right)_{i,M1} ** P_{i,M2} ** \left(P^\dagger\right)_{j,L1} - \mathrm{mat}[G, G, G, L2]\,\left(P^\dagger\right)_{i,R} ** P_{i,R} ** P_{j,L2} - \mathrm{mat}[G, L1, G, G]\,\left(P^\dagger\right)_{i,R} ** P_{i,R} ** \left(P^\dagger\right)_{j,L1}$$

part 5

$$\frac{1}{2}\,\text{mat}[\text{M1, L1, M2, L2}]\,(P^\dagger)_{i,\text{M1}} ** P_{i,\text{M2}} ** (P^\dagger)_{j,\text{L1}} ** P_{j,\text{L2}} - \text{mat}[\text{M1, G, M2, G}]\,(P^\dagger)_{i,\text{M1}} ** P_{i,\text{M2}} ** (P^\dagger)_{j,R} ** P_{j,R} + \frac{1}{2}\,\text{mat}[\text{G, G, G, G}]\,(P^\dagger)_{i,S} ** P_{i,S} ** (P^\dagger)_{j,R} ** P_{j,R}$$

```
(* rename index to show that some terms are actually equivalent *)
Print["part1"]
part1 /. {L1 → M, L2 → M}
Print["part2"]
part2 /. {M2 → M, L2 → L, M1 → M, L1 → L}
Print["part3"]
part3 /. {R → M, M2 → M, L1 → L, M1 → L}
Print["part4"]
part4 /. {M1 → M, L1 → L, M2 → M', L2 → L', R → M}
Print["part5"]
part5 /. {M1 → M, L1 → L, M2 → M', L2 → L', R → L, S → M}
```

part1

$$\frac{1}{2}\,\text{mat}[\text{G, G, G, G}] + \varepsilon_0 + \text{mat}[\text{G, G, G, M}]\,P_{j,M} + \text{mat}[\text{G, M, G, G}]\,(P^\dagger)_{j,M}$$

part2

$$\frac{1}{2}\,\text{mat}[\text{G, G, M, L}]\,P_{i,M} ** P_{j,L} + \frac{1}{2}\,\text{mat}[\text{M, L, G, G}]\,(P^\dagger)_{i,M} ** (P^\dagger)_{j,L}$$

part3

$$\text{mat}[\text{G, L, M, G}]\,P_{i,M} ** (P^\dagger)_{j,L} + \text{mat}[\text{L, G, M, G}]\,(P^\dagger)_{i,L} ** P_{i,M} - \text{mat}[\text{G, G, G, G}]\,(P^\dagger)_{i,M} ** P_{i,M} + (P^\dagger)_{i,M} ** P_{i,M}\,(-\varepsilon_0 + \varepsilon_M)$$

part4

$$\text{mat}[\text{G, L, M}', \text{L}']\,P_{i,M'} ** (P^\dagger)_{j,L} ** P_{j,L'} - \text{mat}[\text{G, G, G, L}']\,(P^\dagger)_{i,M} ** P_{i,M} ** P_{j,L'} - \text{mat}[\text{G, L, G, G}]\,(P^\dagger)_{i,M} ** P_{i,M} ** (P^\dagger)_{j,L} + \text{mat}[\text{M, L, M}', \text{G}]\,(P^\dagger)_{i,M} ** P_{i,M'} ** (P^\dagger)_{j,L}$$

part5

$$\frac{1}{2}\,\text{mat}[\text{G, G, G, G}]\,(P^\dagger)_{i,M} ** P_{i,M} ** (P^\dagger)_{j,L} ** P_{j,L} - \text{mat}[\text{M, G, M}', \text{G}]\,(P^\dagger)_{i,M} ** P_{i,M'} ** (P^\dagger)_{j,L} ** P_{j,L} + \frac{1}{2}\,\text{mat}[\text{M, L, M}', \text{L}']\,(P^\dagger)_{i,M} ** P_{i,M'} ** (P^\dagger)_{j,L} ** P_{j,L'}$$

Part 1 is equivalent to

$N\varepsilon_0 + \frac{1}{2}\sum_{i,j}\langle G, G \mid V_{i,j} \mid G, G\rangle + \sum_{i,j}\sum_M \left[\langle G, G \mid V_{i,j} \mid G, M\rangle P_{j,M} + \langle G, M \mid V_{i,j} \mid G, G\rangle \left(P^\dagger\right)_{j,M}\right]$

rewritten in a more compact way

$E_0 + \sum_j \sum_M \left[A1_M(i, j) P_{j,M} + A2_M(i, j)\left(P^\dagger\right)_{j,M}\right]$

where

$A1_M(i, j) = \sum_i \langle G, G \mid V_{i,j} \mid G, M\rangle$

$A2_M(i, j) = \sum_i \langle G, M \mid V_{i,j} \mid G, G\rangle$

Part 2 is equivalent to

$\frac{1}{2}\sum_{i,j}\sum_{M,L}\left[\langle G, G \mid V_{i,j} \mid M, L\rangle P_{i,M} P_{j,L} + \langle M, L \mid V_{i,j} \mid G, G\rangle \left(P^\dagger\right)_{i,M}\left(P^\dagger\right)_{j,L}\right]$

$= \frac{1}{2}\sum_{i,j}\sum_{M,L}\left[\mathrm{B1}_{M,L}(i, j) P_{i,M} P_{j,L} + \mathrm{B2}_{M,L}(i, j)\left(P^\dagger\right)_{i,M}\left(P^\dagger\right)_{j,L}\right]$

where

$\mathrm{B1}_{M,L}(i, j) = \langle G, G \mid V_{i,j} \mid M, L\rangle$

$\mathrm{B2}_{M,L}(i, j) = \langle M, L \mid V_{i,j} \mid G, G\rangle$

Part 3 is equivalent to

$\sum_{i,j}\sum_{M,L}\langle G, L \mid V_{i,j} \mid M, G\rangle P_{i,M}\left(P^\dagger\right)_{j,L} + \sum_{i,j}\sum_{M,L}\langle L, G \mid V_{i,j} \mid M, G\rangle \left(P^\dagger\right)_{i,L} P_{i,M} +$

$\sum_i \left[-\sum_j \sum_M \langle G, G \mid V_{i,j} \mid G, G\rangle \left(P^\dagger\right)_{i,M} P_{i,M} + \sum_M \left(P^\dagger\right)_{i,M} P_{i,M}(\varepsilon_M - \varepsilon_0)\right]$

$= \sum_{i,j}\sum_{M,L}\langle G, L \mid V_{i,j} \mid M, G\rangle P_{i,M}\left(P^\dagger\right)_{j,L} +$

$\sum_i \left[\sum_j \sum_{M,L}(1 - \delta_{M,L})\langle L, G \mid V_{i,j} \mid M, G\rangle\right]\left(P^\dagger\right)_{i,L} P_{i,M} +$

$\sum_i \sum_M \left[(\varepsilon_M - \varepsilon_0) + \sum_j (\langle M, G \mid V_{i,j} \mid M, G\rangle - \langle G, G \mid V_{i,j} \mid G, G\rangle)\right]\left(P^\dagger\right)_{i,M} P_{i,M}$

$$= \sum_{i,j} \sum_{M,L} \mathrm{B3}_{L,M}(i,\ j)\, P_{i,M} (P^\dagger)_{j,L} + \sum_i \sum_{M,L} \mathrm{B4}_{L,M}(i,\ j) (P^\dagger)_{i,L} P_{i,M} + \sum_i \sum_M \mathrm{B5}_M(i,\ j) (P^\dagger)_{i,M} P_{i,M}$$

where

$\mathrm{B3}_{L,M}(i,\ j) = \langle G, L \mid V_{i,j} \mid M, G \rangle$

$\mathrm{B4}_{L,M}(i,\ j) = \sum_j (1 - \delta_{M,L}) \langle L, G \mid V_{i,j} \mid M, G \rangle$

$\mathrm{B5}_M(i,\ j) = (\varepsilon_M - \varepsilon_0) + \sum_j (\langle M, G \mid V_{i,j} \mid M, G \rangle - \langle G, G \mid V_{i,j} \mid G, G \rangle)$

Part 4 is equivalent to

$$\sum_{i,j} \Big[\sum_{M', L, L'} \langle G, L \mid V_{i,j} \mid M', L' \rangle P_{i,M'} (P^\dagger)_{j,L} P_{j,L'} - \sum_{M, L'} \langle G, G \mid V_{i,j} \mid G, L' \rangle (P^\dagger)_{i,M} P_{i,M} P_{j,L'} - \sum_{M, L} \langle G, L \mid V_{i,j} \mid G, G \rangle (P^\dagger)_{i,M} P_{i,M} (P^\dagger)_{j,L} + \sum_{M', M, L} \langle M, L \mid V_{i,j} \mid M', G \rangle (P^\dagger)_{i,M} P_{i,M'} (P^\dagger)_{j,L} \Big]$$

$$= \sum_{i,j} \Big\{ \sum_{M', L, L'} \langle L, G \mid V_{i,j} \mid L', M' \rangle (P^\dagger)_{i,L} P_{i,L'} P_{j,M'} - \sum_{M, M', L} \delta_{M,M'} \langle G, G \mid V_{i,j} \mid G, L' \rangle (P^\dagger)_{i,M} P_{i,M'} P_{j,L'} + \sum_{M', M, L} [\langle M, L \mid V_{i,j} \mid M', G \rangle - \delta_{M,M'} \langle G, L \mid V_{i,j} \mid G, G \rangle] (P^\dagger)_{i,M} P_{i,M'} (P^\dagger)_{j,L} \Big\}$$

$$= \sum_{i,j} \Big\{ \sum_{M,M', L} [\langle M, G \mid V_{i,j} \mid M', L \rangle - \delta_{M,M'} \langle G, G \mid V_{i,j} \mid G, L \rangle] (P^\dagger)_{i,M} P_{i,M'} P_{j,L} + \sum_{M', M, L} [\langle M, L \mid V_{i,j} \mid M', G \rangle - \delta_{M,M'} \langle G, L \mid V_{i,j} \mid G, G \rangle] (P^\dagger)_{i,M} P_{i,M'} (P^\dagger)_{j,L} \Big\}$$

$$= \sum_{i,j} \Big\{ \sum_{M,M', L} C1_{M, M' L}(i,\ j) (P^\dagger)_{i,M} P_{i,M'} P_{j,L} + \sum_{M', M, L} C2_{\mathrm{ML}, M'}(i,\ j) (P^\dagger)_{i,M} P_{i,M'} (P^\dagger)_{j,L} \Big\}$$

where

$C1_{M, M' L}(i,\ j) = \langle M, G \mid V_{i,j} \mid M', L \rangle - \delta_{M,M'} \langle G, G \mid V_{i,j} \mid G, L \rangle$

$C2_{\mathrm{ML}, M'}(i,\ j) = \langle M, L \mid V_{i,j} \mid M', G \rangle - \delta_{M,M'} \langle G, L \mid V_{i,j} \mid G, G \rangle$

Part 5 is equivalent to

$$\frac{1}{2}\sum_{i,j}\Big[\sum_{M,L}\langle G,G\,|\,V_{i,j}\,|\,G,G\rangle\,\big(P^{\dagger}\big)_{i,M}\,P_{i,M}\big(P^{\dagger}\big)_{j,L}\,P_{j,L} -$$
$$2\sum_{M,M',L}\langle M,G\,|\,V_{i,j}\,|\,M',G\rangle\,\big(P^{\dagger}\big)_{i,M}\,P_{i,M'}\big(P^{\dagger}\big)_{j,L}\,P_{j,L} +$$
$$\sum_{M,M',L,L'}\langle M,L\,|\,V_{i,j}\,|\,M',L'\rangle\,\big(P^{\dagger}\big)_{i,M}\,P_{i,M'}\big(P^{\dagger}\big)_{j,L}\,P_{j,L'}\Big]$$

$$= \frac{1}{2}\sum_{i,j}\sum_{M,M',L,L'}\Big\{\Big[\delta_{M,M'}\,\delta_{L,L'}\,\langle G,G\,|\,V_{i,j}\,|\,G,G\rangle -$$
$$2\,\delta_{L,L'}\,\langle M,G\,|\,V_{i,j}\,|\,M',G\rangle + \langle M,L\,|\,V_{i,j}\,|\,M',L'\rangle\Big]\big(P^{\dagger}\big)_{i,M}\,P_{i,M'}\big(P^{\dagger}\big)_{j,L}\,P_{j,L'}\Big\}$$

$$= \frac{1}{2}\sum_{i,j}\sum_{M,M',L,L'}\Big\{\Big[\delta_{M,M'}\,\delta_{L,L'}\,\langle G,G\,|\,V_{i,j}\,|\,G,G\rangle - 2\,\delta_{L,L'}\,\langle M,G\,|\,V_{i,j}\,|\,M',G\rangle +$$
$$\langle M,L\,|\,V_{i,j}\,|\,M',L'\rangle\Big]\big(P^{\dagger}\big)_{i,M}\,P_{i,M'}\big(P^{\dagger}\big)_{j,L}\,P_{j,L'}\Big\}$$

where

$$D_{\mathrm{ML},M'L'}(i,\ j) =$$
$$\delta_{M,M'}\,\delta_{L,L'}\,\langle G,G\,|\,V_{i,j}\,|\,G,G\rangle - 2\,\delta_{L,L'}\,\langle M,G\,|\,V_{i,j}\,|\,M',G\rangle + \langle M,L\,|\,V_{i,j}\,|\,M',L'\rangle$$