```
ClearAll["Global`*"]
```

```
expand = NonCommutativeMultiply[ x___, Plus[y_, z_, w_], v___] →
   Plus[NonCommutativeMultiply[ x, y, v] +
     NonCommutativeMultiply[x, z, v] + NonCommutativeMultiply[x, w, v]];
```

Test the substititution rule "expand"

```
y ** (a + b + w) ** x /. expand
```

```
y ** a ** x + y ** b ** x + y ** w ** x
```

```
y ** (a + b + w) /. expand
```

```
y ** a + y ** b + y ** w
```

```
(a + b + w) ** y /. expand
```

```
a ** y + b ** y + w ** y
```

```
(a + b + w) ** (m + n + k) //. expand
```

```
a ** k + a ** m + a ** n + b ** k + b ** m + b ** n + w ** k + w ** m + w ** n
```

```
2 ** (i + j + k) ** (u + v + w) ** (x + y + z) ** 9 //. expand
```

```
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 $P^{\dagger}$.

```
(*P and Pdag 's first element is P*)
ourtest[x_] :=
 If[( (Length[x] == 1) && (x[[1]] =!= P) ) || IntegerQ[x] || (x[[1]] == δ), True, False]
(* when you use && and ||, remember to add brackets!!*)
clean =
 NonCommutativeMultiply[x___, u_ /; ourtest[u], y___] :>
  Times[NonCommutativeMultiply[x, y], u];
(* we want to get rid of "**" in places where they are not supposed to appear *)
```

Test the substitution rule "clean"

$(P^{\dagger})_m ** P_n ** P_m ** (P^{\dagger})_{n1}$ //. clean

$(P^{\dagger})_m ** P_n ** P_m ** (P^{\dagger})_{n1}$

$(P^{\dagger})_m ** P_n ** P_m ** (P^{\dagger})_{n1} ** (-2)$ //. clean

$-2\ (P^{\dagger})_m ** P_n ** P_m ** (P^{\dagger})_{n1}$

$(P^{\dagger})_m ** P_n ** P_m ** (-2) ** (P^{\dagger})_{n1}$ //. clean

$-2\ (P^{\dagger})_m ** P_n ** P_m ** (P^{\dagger})_{n1}$

$2 ** (P^{\dagger})_m ** P_n ** P_m ** (P^{\dagger})_{n1}$ //. clean

$2\ (P^{\dagger})_m ** P_n ** P_m ** (P^{\dagger})_{n1}$

$(P^{\dagger})_m ** P_n ** \delta_{m,n1} ** P_m ** (P^{\dagger})_{n1}$ //. clean

$(P^{\dagger})_m ** P_n ** P_m ** (P^{\dagger})_{n1}\ \delta_{m,n1}$

```
(P†)_m ** 7 ** P_n ** δ_{m,n1} ** P_m ** 2 ** (P†)_n1 //. clean
```

```
14 (P†)_m ** P_n ** P_m ** (P†)_n1 δ_{m,n1}
```

```
deletezero = NonCommutativeMultiply[x___, P_] → 0
```

```
x___ ** P_ → 0
```

Test the above rule

```
4 (P†)_n ** (P†)_n ** (P†)_n ** P_n ϵ_0 δ_{n,m} δ_{n,n1} δ_{n,n2} c_{n1,n2,n3} /. deletezero
```

```
0
```

```
(P†)_n ** (P†)_m ** P_n ** (P†)_n1 ** P_m ** (P†)_n2 ** (P†)_n3 /. deletezero
```

```
0 ** (P†)_n2 ** (P†)_n3
```

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

```
Replace[(P†)_n ** (P†)_m ** P_n ** (P†)_n1 ** P_m ** (P†)_n2 ** (P†)_n3, deletezero, 1]
```

```
(P†)_n ** (P†)_m ** P_n ** (P†)_n1 ** P_m ** (P†)_n2 ** (P†)_n3
```

```
Replace[4 (P†)_n ** (P†)_n ** (P†)_n ** P_n ϵ_0 δ_{n,m} δ_{n,n1} δ_{n,n2} c_{n1,n2,n3}, deletezero, 1]
```

```
0
```

```
Replace[4 (P†)n ** (P†)n ** (P†)n ** Pn ϵ0 δn,m δn,n1 δn,n2 Cn1,n2,n3 +
  (P†)n ** (P†)m ** Pn ** (P†)n1 ** Pm ** (P†)n2 ** (P†)n3, deletezero, 1]
```

```
(P†)n ** (P†)m ** Pn ** (P†)n1 ** Pm ** (P†)n2 ** (P†)n3 +
 4 (P†)n ** (P†)n ** (P†)n ** Pn ϵ0 δn,m δn,n1 δn,n2 Cn1,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

```
deleteZeroTerm[x_] := Module[
  {xlist},
  xlist = Apply[List, x] ; (*divide a single term into a list*)
  Do[
   xlist[[i]] = Replace[xlist[[i]], deletezero, 1],
   {i, 1, Length[xlist]}
  ];
  Apply[Plus, xlist]
 ]
```

```
deleteZeroTerm[4 (P†)n ** (P†)n ** (P†)n ** Pn ϵ0 δn,m δn,n1 δn,n2 Cn1,n2,n3 +
  (P†)n ** (P†)m ** Pn ** (P†)n1 ** Pm ** (P†)n2 ** (P†)n3]
```

```
(P†)n ** (P†)m ** Pn ** (P†)n1 ** Pm ** (P†)n2 ** (P†)n3
```

Schrodinger equation takinng into account of kinematic interaction

```
(* multiply two terms,
each term may contain both Times and NonCommutativeMultiply *)
multiply[x_, y_] := Which[
  MatchQ[x, NonCommutativeMultiply[_]] && MatchQ[y, NonCommutativeMultiply[_]], x ** y,

  MatchQ[x, Times[_]] && MatchQ[y, NonCommutativeMultiply[_]],
  x ** y /. Times[u__, NonCommutativeMultiply[v_]] ** NonCommutativeMultiply[w_] →
    Times[u, NonCommutativeMultiply[v, w]],

   MatchQ[x, Times[_]] && MatchQ[y, Times[_]], x ** y /.
   Times[u__, NonCommutativeMultiply[v_]] ** Times[q__, NonCommutativeMultiply[w_]] →
    Times[u, q, NonCommutativeMultiply[v, w]]
 ]
```

```
(* define operators for the convenience of writing *)
Pdag[x_] := (P†)x;
P[x_] := Px;
delta[x_, y_] := δx,y
c[n1_, n2_, n3_] := cn1,n2,n3
```

The commutation relation between two operators can be written as

```
commutationRule =
 P[a_] ** Pdag[b_] → delta[a, b] + Pdag[b] ** P[a] + (-2) ** delta[a, b] ** Pdag[a] ** P[a]
(* writing in terms of (-2) will save us some trouble *)
(* it is better to regard all multiplication as noncommutative *)
```

$P_{a\_} ** (P^\dagger)_{b\_} \to (P^\dagger)_b ** P_a + (-2) ** \delta_{a,b} ** (P^\dagger)_a ** P_a + \delta_{a,b}$

the Hamiltonian including the dynamical interaction is

```
ham = Sum[ϵ0 Pdag[n] ** P[n], n] + Sum[Sum[jexn,m Pdag[n] ** P[m], n], m] +
  1/2 Sum[Sum[dynn,m Pdag[n] ** P[n] ** Pdag[m] ** P[m], n], m]
```

$$\sum_n (P^\dagger)_n ** P_n \,\epsilon_0 + \frac{1}{2} \sum_m \left(\sum_n (P^\dagger)_n ** P_n ** (P^\dagger)_m ** P_m \, \mathrm{dyn}_{n,m} \right) + \sum_m \left(\sum_n (P^\dagger)_n ** P_m \, \mathrm{jex}_{n,m} \right)$$

in order to simplify the derivation, we will ignore the summmation of n and m, then the hamiltonian can be written as

```
ham = (*delta[n,m]*)
 ϵ0 Pdag[n] ** P[n] + jexn,m Pdag[n] ** P[m] + 1/2 dynn,m Pdag[n] ** P[n] ** Pdag[m] ** P[m]
```

$$(P^\dagger)_n ** P_n \,\epsilon_0 + \frac{1}{2} (P^\dagger)_n ** P_n ** (P^\dagger)_m ** P_m \, \mathrm{dyn}_{n,m} + (P^\dagger)_n ** P_m \, \mathrm{jex}_{n,m}$$

Note that the term with ϵ_0 is a single summation over n

The three-exciton state is given by (the vaccum state is ignored here)

```
Sum[
 Sum[
  Sum[c[n1, n2, n3] Pdag[n1] ** Pdag[n2] ** Pdag[n3], n1], n2],
 n3]
```

$$\sum_{n3} \left(\sum_{n2} \left(\sum_{n1} (P^\dagger)_{n1} ** (P^\dagger)_{n2} ** (P^\dagger)_{n3} \, c_{n1,n2,n3} \right) \right)$$

For simplicity, we ignore the summations in the above three-exciton state and let the hamiltonian operate on it. (the coefficient c will be dropped for a moment)

```
threeExciton = Pdag[n1] ** Pdag[n2] ** Pdag[n3] c[n1, n2, n3]
```

$(P^\dagger)_{n1} ** (P^\dagger)_{n2} ** (P^\dagger)_{n3} \, c_{n1,n2,n3}$

In the following, the left-hand side is $H \mid \psi\rangle$

```
lhs = Apply[
  Plus,
  Table[multiply[ham[[i]], threeExciton], {i, 1, Length[ham]}]
 ]
```

$$(P^\dagger)_n ** P_n ** (P^\dagger)_{n1} ** (P^\dagger)_{n2} ** (P^\dagger)_{n3}\, \epsilon_0\, C_{n1,n2,n3} + \frac{1}{2} (P^\dagger)_n ** P_n ** (P^\dagger)_m ** P_m ** (P^\dagger)_{n1} ** (P^\dagger)_{n2} ** (P^\dagger)_{n3}\, \mathrm{dyn}_{n,m}\, C_{n1,n2,n3} + (P^\dagger)_n ** P_m ** (P^\dagger)_{n1} ** (P^\dagger)_{n2} ** (P^\dagger)_{n3}\, \mathrm{jex}_{n,m}\, C_{n1,n2,n3}$$

Let's treate the first term separately (see "Dealing with the first term in the hamiltonian")

```
lhs0 = First[lhs]
```

$$(P^\dagger)_n ** P_n ** (P^\dagger)_{n1} ** (P^\dagger)_{n2} ** (P^\dagger)_{n3}\, \epsilon_0\, C_{n1,n2,n3}$$

Dealing with the first term in the hamiltonian

```
lhs01 = lhs0 //. commutationRule //. expand // ExpandAll
```

$$(P^\dagger)_n ** \delta_{n,n1} ** (P^\dagger)_{n2} ** (P^\dagger)_{n3}\, \epsilon_0\, C_{n1,n2,n3} + (P^\dagger)_n ** (P^\dagger)_{n1} ** P_n ** (P^\dagger)_{n2} ** (P^\dagger)_{n3}\, \epsilon_0\, C_{n1,n2,n3} + (P^\dagger)_n ** (-2) ** \delta_{n,n1} ** (P^\dagger)_n ** P_n ** (P^\dagger)_{n2} ** (P^\dagger)_{n3}\, \epsilon_0\, C_{n1,n2,n3}$$

```
lhs02 = lhs01 //. clean
```

$$(P^\dagger)_n ** (P^\dagger)_{n1} ** P_n ** (P^\dagger)_{n2} ** (P^\dagger)_{n3}\, \epsilon_0\, C_{n1,n2,n3} + (P^\dagger)_n ** (P^\dagger)_{n2} ** (P^\dagger)_{n3}\, \epsilon_0\, \delta_{n,n1}\, C_{n1,n2,n3} - 2\, (P^\dagger)_n ** (P^\dagger)_n ** P_n ** (P^\dagger)_{n2} ** (P^\dagger)_{n3}\, \epsilon_0\, \delta_{n,n1}\, C_{n1,n2,n3}$$

```
lhs03 = lhs02 //. commutationRule //. expand // ExpandAll
```

$$(P^\dagger)_n ** (P^\dagger)_{n1} ** \delta_{n,n2} ** (P^\dagger)_{n3}\, \epsilon_0\, C_{n1,n2,n3} + (P^\dagger)_n ** (P^\dagger)_{n1} ** (P^\dagger)_{n2} ** P_n ** (P^\dagger)_{n3}\, \epsilon_0\, C_{n1,n2,n3} + (P^\dagger)_n ** (P^\dagger)_{n1} ** (-2) ** \delta_{n,n2} ** (P^\dagger)_n ** P_n ** (P^\dagger)_{n3}\, \epsilon_0\, C_{n1,n2,n3} + (P^\dagger)_n ** (P^\dagger)_{n2} ** (P^\dagger)_{n3}\, \epsilon_0\, \delta_{n,n1}\, C_{n1,n2,n3} - 2\, (P^\dagger)_n ** (P^\dagger)_n ** \delta_{n,n2} ** (P^\dagger)_{n3}\, \epsilon_0\, \delta_{n,n1}\, C_{n1,n2,n3} - 2\, (P^\dagger)_n ** (P^\dagger)_n ** (P^\dagger)_{n2} ** P_n ** (P^\dagger)_{n3}\, \epsilon_0\, \delta_{n,n1}\, C_{n1,n2,n3} - 2\, (P^\dagger)_n ** (P^\dagger)_n ** (-2) ** \delta_{n,n2} ** (P^\dagger)_n ** P_n ** (P^\dagger)_{n3}\, \epsilon_0\, \delta_{n,n1}\, C_{n1,n2,n3}$$

```
lhs04 = lhs03 //. clean
```

$$(P^\dagger)_n ** (P^\dagger)_{n1} ** (P^\dagger)_{n2} ** P_n ** (P^\dagger)_{n3}\, \epsilon_0\, C_{n1,n2,n3} + (P^\dagger)_n ** (P^\dagger)_{n2} ** (P^\dagger)_{n3}\, \epsilon_0\, \delta_{n,n1}\, C_{n1,n2,n3} - 2\, (P^\dagger)_n ** (P^\dagger)_n ** (P^\dagger)_{n2} ** P_n ** (P^\dagger)_{n3}\, \epsilon_0\, \delta_{n,n1}\, C_{n1,n2,n3} + (P^\dagger)_n ** (P^\dagger)_{n1} ** (P^\dagger)_{n3}\, \epsilon_0\, \delta_{n,n2}\, C_{n1,n2,n3} - 2\, (P^\dagger)_n ** (P^\dagger)_{n1} ** (P^\dagger)_n ** P_n ** (P^\dagger)_{n3}\, \epsilon_0\, \delta_{n,n2}\, C_{n1,n2,n3} - 2\, (P^\dagger)_n ** (P^\dagger)_n ** (P^\dagger)_{n3}\, \epsilon_0\, \delta_{n,n1}\, \delta_{n,n2}\, C_{n1,n2,n3} + 4\, (P^\dagger)_n ** (P^\dagger)_n ** (P^\dagger)_n ** P_n ** (P^\dagger)_{n3}\, \epsilon_0\, \delta_{n,n1}\, \delta_{n,n2}\, C_{n1,n2,n3}$$

lhs05 = lhs04 //. commutationRule //. expand // ExpandAll

$$\begin{aligned}
&(P^\dagger)_n ** (P^\dagger)_{n1} ** (P^\dagger)_{n2} ** \delta_{n,n3}\,\epsilon_0\, C_{n1,n2,n3} + (P^\dagger)_n ** (P^\dagger)_{n1} ** (P^\dagger)_{n2} ** (P^\dagger)_{n3} ** P_n\,\epsilon_0\, C_{n1,n2,n3} + \\
&(P^\dagger)_n ** (P^\dagger)_{n1} ** (P^\dagger)_{n2} ** (-2) ** \delta_{n,n3} ** (P^\dagger)_n ** P_n\,\epsilon_0\, C_{n1,n2,n3} + \\
&(P^\dagger)_n ** (P^\dagger)_{n2} ** (P^\dagger)_{n3}\,\epsilon_0\,\delta_{n,n1}\, C_{n1,n2,n3} - 2\,(P^\dagger)_n ** (P^\dagger)_n ** (P^\dagger)_{n2} ** \delta_{n,n3}\,\epsilon_0\,\delta_{n,n1}\, C_{n1,n2,n3} - \\
&2\,(P^\dagger)_n ** (P^\dagger)_n ** (P^\dagger)_{n2} ** (P^\dagger)_{n3} ** P_n\,\epsilon_0\,\delta_{n,n1}\, C_{n1,n2,n3} - \\
&2\,(P^\dagger)_n ** (P^\dagger)_n ** (P^\dagger)_{n2} ** (-2) ** \delta_{n,n3} ** (P^\dagger)_n ** P_n\,\epsilon_0\,\delta_{n,n1}\, C_{n1,n2,n3} + \\
&(P^\dagger)_n ** (P^\dagger)_{n1} ** (P^\dagger)_{n3}\,\epsilon_0\,\delta_{n,n2}\, C_{n1,n2,n3} - 2\,(P^\dagger)_n ** (P^\dagger)_{n1} ** (P^\dagger)_n ** \delta_{n,n3}\,\epsilon_0\,\delta_{n,n2}\, C_{n1,n2,n3} - \\
&2\,(P^\dagger)_n ** (P^\dagger)_{n1} ** (P^\dagger)_n ** (P^\dagger)_{n3} ** P_n\,\epsilon_0\,\delta_{n,n2}\, C_{n1,n2,n3} - \\
&2\,(P^\dagger)_n ** (P^\dagger)_{n1} ** (P^\dagger)_n ** (-2) ** \delta_{n,n3} ** (P^\dagger)_n ** P_n\,\epsilon_0\,\delta_{n,n2}\, C_{n1,n2,n3} - \\
&2\,(P^\dagger)_n ** (P^\dagger)_n ** (P^\dagger)_{n3}\,\epsilon_0\,\delta_{n,n1}\,\delta_{n,n2}\, C_{n1,n2,n3} + \\
&4\,(P^\dagger)_n ** (P^\dagger)_n ** (P^\dagger)_n ** \delta_{n,n3}\,\epsilon_0\,\delta_{n,n1}\,\delta_{n,n2}\, C_{n1,n2,n3} + \\
&4\,(P^\dagger)_n ** (P^\dagger)_n ** (P^\dagger)_n ** (P^\dagger)_{n3} ** P_n\,\epsilon_0\,\delta_{n,n1}\,\delta_{n,n2}\, C_{n1,n2,n3} + \\
&4\,(P^\dagger)_n ** (P^\dagger)_n ** (P^\dagger)_n ** (-2) ** \delta_{n,n3} ** (P^\dagger)_n ** P_n\,\epsilon_0\,\delta_{n,n1}\,\delta_{n,n2}\, C_{n1,n2,n3}
\end{aligned}$$

lhs06 = lhs05 //. clean

$$\begin{aligned}
&(P^\dagger)_n ** (P^\dagger)_{n1} ** (P^\dagger)_{n2} ** (P^\dagger)_{n3} ** P_n\,\epsilon_0\, C_{n1,n2,n3} + \\
&(P^\dagger)_n ** (P^\dagger)_{n2} ** (P^\dagger)_{n3}\,\epsilon_0\,\delta_{n,n1}\, C_{n1,n2,n3} - 2\,(P^\dagger)_n ** (P^\dagger)_n ** (P^\dagger)_{n2} ** (P^\dagger)_{n3} ** P_n\,\epsilon_0\,\delta_{n,n1}\, C_{n1,n2,n3} + \\
&(P^\dagger)_n ** (P^\dagger)_{n1} ** (P^\dagger)_{n3}\,\epsilon_0\,\delta_{n,n2}\, C_{n1,n2,n3} - 2\,(P^\dagger)_n ** (P^\dagger)_{n1} ** (P^\dagger)_n ** (P^\dagger)_{n3} ** P_n\,\epsilon_0\,\delta_{n,n2}\, C_{n1,n2,n3} - \\
&2\,(P^\dagger)_n ** (P^\dagger)_n ** (P^\dagger)_{n3}\,\epsilon_0\,\delta_{n,n1}\,\delta_{n,n2}\, C_{n1,n2,n3} + \\
&4\,(P^\dagger)_n ** (P^\dagger)_n ** (P^\dagger)_n ** (P^\dagger)_{n3} ** P_n\,\epsilon_0\,\delta_{n,n1}\,\delta_{n,n2}\, C_{n1,n2,n3} + \\
&(P^\dagger)_n ** (P^\dagger)_{n1} ** (P^\dagger)_{n2}\,\epsilon_0\,\delta_{n,n3}\, C_{n1,n2,n3} - 2\,(P^\dagger)_n ** (P^\dagger)_{n1} ** (P^\dagger)_{n2} ** (P^\dagger)_n ** P_n\,\epsilon_0\,\delta_{n,n3}\, C_{n1,n2,n3} - \\
&2\,(P^\dagger)_n ** (P^\dagger)_n ** (P^\dagger)_{n2}\,\epsilon_0\,\delta_{n,n1}\,\delta_{n,n3}\, C_{n1,n2,n3} + \\
&4\,(P^\dagger)_n ** (P^\dagger)_n ** (P^\dagger)_{n2} ** (P^\dagger)_n ** P_n\,\epsilon_0\,\delta_{n,n1}\,\delta_{n,n3}\, C_{n1,n2,n3} - \\
&2\,(P^\dagger)_n ** (P^\dagger)_{n1} ** (P^\dagger)_n\,\epsilon_0\,\delta_{n,n2}\,\delta_{n,n3}\, C_{n1,n2,n3} + \\
&4\,(P^\dagger)_n ** (P^\dagger)_{n1} ** (P^\dagger)_n ** (P^\dagger)_n ** P_n\,\epsilon_0\,\delta_{n,n2}\,\delta_{n,n3}\, C_{n1,n2,n3} + \\
&4\,(P^\dagger)_n ** (P^\dagger)_n ** (P^\dagger)_n\,\epsilon_0\,\delta_{n,n1}\,\delta_{n,n2}\,\delta_{n,n3}\, C_{n1,n2,n3} - \\
&8\,(P^\dagger)_n ** (P^\dagger)_n ** (P^\dagger)_n ** (P^\dagger)_n ** P_n\,\epsilon_0\,\delta_{n,n1}\,\delta_{n,n2}\,\delta_{n,n3}\, C_{n1,n2,n3}
\end{aligned}$$

lhs07 = deleteZeroTerm[lhs06]

$$\begin{aligned}
&(P^\dagger)_n ** (P^\dagger)_{n2} ** (P^\dagger)_{n3}\,\epsilon_0\,\delta_{n,n1}\, C_{n1,n2,n3} + \\
&(P^\dagger)_n ** (P^\dagger)_{n1} ** (P^\dagger)_{n3}\,\epsilon_0\,\delta_{n,n2}\, C_{n1,n2,n3} - 2\,(P^\dagger)_n ** (P^\dagger)_n ** (P^\dagger)_{n3}\,\epsilon_0\,\delta_{n,n1}\,\delta_{n,n2}\, C_{n1,n2,n3} + \\
&(P^\dagger)_n ** (P^\dagger)_{n1} ** (P^\dagger)_{n2}\,\epsilon_0\,\delta_{n,n3}\, C_{n1,n2,n3} - 2\,(P^\dagger)_n ** (P^\dagger)_n ** (P^\dagger)_{n2}\,\epsilon_0\,\delta_{n,n1}\,\delta_{n,n3}\, C_{n1,n2,n3} - \\
&2\,(P^\dagger)_n ** (P^\dagger)_{n1} ** (P^\dagger)_n\,\epsilon_0\,\delta_{n,n2}\,\delta_{n,n3}\, C_{n1,n2,n3} + 4\,(P^\dagger)_n ** (P^\dagger)_n ** (P^\dagger)_n\,\epsilon_0\,\delta_{n,n1}\,\delta_{n,n2}\,\delta_{n,n3}\, C_{n1,n2,n3}
\end{aligned}$$

The above term is within the summation over n, the term with two and three deltas will be zero because you cannot excite a molecule more than once (you will obtain $C_{n1,n1,n3}$, $C_{n1,n2,n2}$, ... etc, which doesn't exist)

lhs08 = lhs07 /. $\{\delta_{n\_,n1\_}\,\delta_{n\_,n3\_} \to 0,\ \delta_{n\_,n1\_}\,\delta_{n\_,n2\_}\,\delta_{n\_,n3\_} \to 0\}$

$$\begin{aligned}
&(P^\dagger)_n ** (P^\dagger)_{n2} ** (P^\dagger)_{n3}\,\epsilon_0\,\delta_{n,n1}\, C_{n1,n2,n3} + \\
&(P^\dagger)_n ** (P^\dagger)_{n1} ** (P^\dagger)_{n3}\,\epsilon_0\,\delta_{n,n2}\, C_{n1,n2,n3} + (P^\dagger)_n ** (P^\dagger)_{n1} ** (P^\dagger)_{n2}\,\epsilon_0\,\delta_{n,n3}\, C_{n1,n2,n3}
\end{aligned}$$

Put the above term into the summation over n, they are the same, and the total results becomes:

lhs09 = $\mathbf{(P^\dagger)_{n1} ** (P^\dagger)_{n2} ** (P^\dagger)_{n3}\, 3\,\epsilon_0\, C_{n1,n2,n3}}$

$$3\,(P^\dagger)_{n1} ** (P^\dagger)_{n2} ** (P^\dagger)_{n3}\,\epsilon_0\, C_{n1,n2,n3}$$

Dealing with the rest terms in the hamiltonian

```
lhs2 = Rest[lhs] /. commutationRule
```

$$\frac{1}{2}(P^\dagger)_n ** ((P^\dagger)_m ** P_n + (-2) ** \delta_{n,m} ** (P^\dagger)_n ** P_n + \delta_{n,m}) ** P_m ** (P^\dagger)_{n1} ** (P^\dagger)_{n2} ** (P^\dagger)_{n3} \, dyn_{n,m} \, c_{n1,n2,n3} + (P^\dagger)_n ** ((P^\dagger)_{n1} ** P_m + (-2) ** \delta_{m,n1} ** (P^\dagger)_m ** P_m + \delta_{m,n1}) ** (P^\dagger)_{n2} ** (P^\dagger)_{n3} \, jex_{n,m} \, c_{n1,n2,n3}$$

```
lhs3 = lhs2 //. expand
```

$$\frac{1}{2}((P^\dagger)_n ** \delta_{n,m} ** P_m ** (P^\dagger)_{n1} ** (P^\dagger)_{n2} ** (P^\dagger)_{n3} + (P^\dagger)_n ** (P^\dagger)_m ** P_n ** P_m ** (P^\dagger)_{n1} ** (P^\dagger)_{n2} ** (P^\dagger)_{n3} + (P^\dagger)_n ** (-2) ** \delta_{n,m} ** (P^\dagger)_n ** P_n ** P_m ** (P^\dagger)_{n1} ** (P^\dagger)_{n2} ** (P^\dagger)_{n3}) \, dyn_{n,m} \, c_{n1,n2,n3} + ((P^\dagger)_n ** \delta_{m,n1} ** (P^\dagger)_{n2} ** (P^\dagger)_{n3} + (P^\dagger)_n ** (P^\dagger)_{n1} ** P_m ** (P^\dagger)_{n2} ** (P^\dagger)_{n3} + (P^\dagger)_n ** (-2) ** \delta_{m,n1} ** (P^\dagger)_m ** P_m ** (P^\dagger)_{n2} ** (P^\dagger)_{n3}) \, jex_{n,m} \, c_{n1,n2,n3}$$

```
lhs4 = ExpandAll[lhs3]
```

$$\frac{1}{2}(P^\dagger)_n ** \delta_{n,m} ** P_m ** (P^\dagger)_{n1} ** (P^\dagger)_{n2} ** (P^\dagger)_{n3} \, dyn_{n,m} \, c_{n1,n2,n3} + \frac{1}{2}(P^\dagger)_n ** (P^\dagger)_m ** P_n ** P_m ** (P^\dagger)_{n1} ** (P^\dagger)_{n2} ** (P^\dagger)_{n3} \, dyn_{n,m} \, c_{n1,n2,n3} + \frac{1}{2}(P^\dagger)_n ** (-2) ** \delta_{n,m} ** (P^\dagger)_n ** P_n ** P_m ** (P^\dagger)_{n1} ** (P^\dagger)_{n2} ** (P^\dagger)_{n3} \, dyn_{n,m} \, c_{n1,n2,n3} + (P^\dagger)_n ** \delta_{m,n1} ** (P^\dagger)_{n2} ** (P^\dagger)_{n3} \, jex_{n,m} \, c_{n1,n2,n3} + (P^\dagger)_n ** (P^\dagger)_{n1} ** P_m ** (P^\dagger)_{n2} ** (P^\dagger)_{n3} \, jex_{n,m} \, c_{n1,n2,n3} + (P^\dagger)_n ** (-2) ** \delta_{m,n1} ** (P^\dagger)_m ** P_m ** (P^\dagger)_{n2} ** (P^\dagger)_{n3} \, jex_{n,m} \, c_{n1,n2,n3}$$

```
lhs5 = lhs4 //. clean
```

$$\frac{1}{2}(P^\dagger)_n ** (P^\dagger)_m ** P_n ** P_m ** (P^\dagger)_{n1} ** (P^\dagger)_{n2} ** (P^\dagger)_{n3} \, dyn_{n,m} \, c_{n1,n2,n3} + (P^\dagger)_n ** (P^\dagger)_{n1} ** P_m ** (P^\dagger)_{n2} ** (P^\dagger)_{n3} \, jex_{n,m} \, c_{n1,n2,n3} + (P^\dagger)_n ** (P^\dagger)_{n2} ** (P^\dagger)_{n3} \, jex_{n,m} \, \delta_{m,n1} \, c_{n1,n2,n3} - 2 (P^\dagger)_n ** (P^\dagger)_m ** P_m ** (P^\dagger)_{n2} ** (P^\dagger)_{n3} \, jex_{n,m} \, \delta_{m,n1} \, c_{n1,n2,n3} + \frac{1}{2}(P^\dagger)_n ** P_m ** (P^\dagger)_{n1} ** (P^\dagger)_{n2} ** (P^\dagger)_{n3} \, dyn_{n,m} \, \delta_{n,m} \, c_{n1,n2,n3} - (P^\dagger)_n ** (P^\dagger)_n ** P_n ** P_m ** (P^\dagger)_{n1} ** (P^\dagger)_{n2} ** (P^\dagger)_{n3} \, dyn_{n,m} \, \delta_{n,m} \, c_{n1,n2,n3}$$

```
lhs6 = lhs5 //. commutationRule
```

$$\frac{1}{2}\left(P^{\dagger}\right)_{n}**\left(P^{\dagger}\right)_{m}**P_{n}**\left(\left(\left(P^{\dagger}\right)_{n1}**P_{m}+(-2)**\delta_{m,n1}**\left(P^{\dagger}\right)_{m}**P_{m}+\delta_{m,n1}\right)**\left(P^{\dagger}\right)_{n2}**\left(P^{\dagger}\right)_{n3}\,\mathrm{dyn}_{n,m}\,c_{n1,n2,n3}+\left(P^{\dagger}\right)_{n}**\left(P^{\dagger}\right)_{n1}**\left(\left(P^{\dagger}\right)_{n2}**P_{m}+(-2)**\delta_{m,n2}**\left(P^{\dagger}\right)_{m}**P_{m}+\delta_{m,n2}\right)**\left(P^{\dagger}\right)_{n3}\,\mathrm{jex}_{n,m}\,c_{n1,n2,n3}+\left(P^{\dagger}\right)_{n}**\left(P^{\dagger}\right)_{n2}**\left(P^{\dagger}\right)_{n3}\,\mathrm{jex}_{n,m}\,\delta_{m,n1}\,c_{n1,n2,n3}-2\left(P^{\dagger}\right)_{n}**\left(P^{\dagger}\right)_{m}**\left(\left(P^{\dagger}\right)_{n2}**P_{m}+(-2)**\delta_{m,n2}**\left(P^{\dagger}\right)_{m}**P_{m}+\delta_{m,n2}\right)**\left(P^{\dagger}\right)_{n3}\,\mathrm{jex}_{n,m}\,\delta_{m,n1}\,c_{n1,n2,n3}+\frac{1}{2}\left(P^{\dagger}\right)_{n}**\left(\left(P^{\dagger}\right)_{n1}**P_{m}+(-2)**\delta_{m,n1}**\left(P^{\dagger}\right)_{m}**P_{m}+\delta_{m,n1}\right)**\left(P^{\dagger}\right)_{n2}**\left(P^{\dagger}\right)_{n3}\,\mathrm{dyn}_{n,m}\,\delta_{n,m}\,c_{n1,n2,n3}-\left(P^{\dagger}\right)_{n}**\left(P^{\dagger}\right)_{n}**P_{n}**\left(\left(P^{\dagger}\right)_{n1}**P_{m}+(-2)**\delta_{m,n1}**\left(P^{\dagger}\right)_{m}**P_{m}+\delta_{m,n1}\right)**\left(P^{\dagger}\right)_{n2}**\left(P^{\dagger}\right)_{n3}\,\mathrm{dyn}_{n,m}\,\delta_{n,m}\,c_{n1,n2,n3}$$

```
lhs7 = ExpandAll[lhs6 //. expand]
```

$$\frac{1}{2}\left(P^{\dagger}\right)_{n}**\left(P^{\dagger}\right)_{m}**P_{n}**\delta_{m,n1}**\left(P^{\dagger}\right)_{n2}**\left(P^{\dagger}\right)_{n3}\,\mathrm{dyn}_{n,m}\,c_{n1,n2,n3}+$$
$$\frac{1}{2}\left(P^{\dagger}\right)_{n}**\left(P^{\dagger}\right)_{m}**P_{n}**\left(P^{\dagger}\right)_{n1}**P_{m}**\left(P^{\dagger}\right)_{n2}**\left(P^{\dagger}\right)_{n3}\,\mathrm{dyn}_{n,m}\,c_{n1,n2,n3}+$$
$$\frac{1}{2}\left(P^{\dagger}\right)_{n}**\left(P^{\dagger}\right)_{m}**P_{n}**(-2)**\delta_{m,n1}**\left(P^{\dagger}\right)_{m}**P_{m}**\left(P^{\dagger}\right)_{n2}**\left(P^{\dagger}\right)_{n3}\,\mathrm{dyn}_{n,m}\,c_{n1,n2,n3}+$$
$$\left(P^{\dagger}\right)_{n}**\left(P^{\dagger}\right)_{n1}**\delta_{m,n2}**\left(P^{\dagger}\right)_{n3}\,\mathrm{jex}_{n,m}\,c_{n1,n2,n3}+$$
$$\left(P^{\dagger}\right)_{n}**\left(P^{\dagger}\right)_{n1}**\left(P^{\dagger}\right)_{n2}**P_{m}**\left(P^{\dagger}\right)_{n3}\,\mathrm{jex}_{n,m}\,c_{n1,n2,n3}+$$
$$\left(P^{\dagger}\right)_{n}**\left(P^{\dagger}\right)_{n1}**(-2)**\delta_{m,n2}**\left(P^{\dagger}\right)_{m}**P_{m}**\left(P^{\dagger}\right)_{n3}\,\mathrm{jex}_{n,m}\,c_{n1,n2,n3}+$$
$$\left(P^{\dagger}\right)_{n}**\left(P^{\dagger}\right)_{n2}**\left(P^{\dagger}\right)_{n3}\,\mathrm{jex}_{n,m}\,\delta_{m,n1}\,c_{n1,n2,n3}-2\left(P^{\dagger}\right)_{n}**\left(P^{\dagger}\right)_{m}**\delta_{m,n2}**\left(P^{\dagger}\right)_{n3}\,\mathrm{jex}_{n,m}\,\delta_{m,n1}\,c_{n1,n2,n3}-$$
$$2\left(P^{\dagger}\right)_{n}**\left(P^{\dagger}\right)_{m}**\left(P^{\dagger}\right)_{n2}**P_{m}**\left(P^{\dagger}\right)_{n3}\,\mathrm{jex}_{n,m}\,\delta_{m,n1}\,c_{n1,n2,n3}-$$
$$2\left(P^{\dagger}\right)_{n}**\left(P^{\dagger}\right)_{m}**(-2)**\delta_{m,n2}**\left(P^{\dagger}\right)_{m}**P_{m}**\left(P^{\dagger}\right)_{n3}\,\mathrm{jex}_{n,m}\,\delta_{m,n1}\,c_{n1,n2,n3}+$$
$$\frac{1}{2}\left(P^{\dagger}\right)_{n}**\delta_{m,n1}**\left(P^{\dagger}\right)_{n2}**\left(P^{\dagger}\right)_{n3}\,\mathrm{dyn}_{n,m}\,\delta_{n,m}\,c_{n1,n2,n3}+$$
$$\frac{1}{2}\left(P^{\dagger}\right)_{n}**\left(P^{\dagger}\right)_{n1}**P_{m}**\left(P^{\dagger}\right)_{n2}**\left(P^{\dagger}\right)_{n3}\,\mathrm{dyn}_{n,m}\,\delta_{n,m}\,c_{n1,n2,n3}-$$
$$\left(P^{\dagger}\right)_{n}**\left(P^{\dagger}\right)_{n}**P_{n}**\delta_{m,n1}**\left(P^{\dagger}\right)_{n2}**\left(P^{\dagger}\right)_{n3}\,\mathrm{dyn}_{n,m}\,\delta_{n,m}\,c_{n1,n2,n3}+$$
$$\frac{1}{2}\left(P^{\dagger}\right)_{n}**(-2)**\delta_{m,n1}**\left(P^{\dagger}\right)_{m}**P_{m}**\left(P^{\dagger}\right)_{n2}**\left(P^{\dagger}\right)_{n3}\,\mathrm{dyn}_{n,m}\,\delta_{n,m}\,c_{n1,n2,n3}-$$
$$\left(P^{\dagger}\right)_{n}**\left(P^{\dagger}\right)_{n}**P_{n}**\left(P^{\dagger}\right)_{n1}**P_{m}**\left(P^{\dagger}\right)_{n2}**\left(P^{\dagger}\right)_{n3}\,\mathrm{dyn}_{n,m}\,\delta_{n,m}\,c_{n1,n2,n3}-$$
$$\left(P^{\dagger}\right)_{n}**\left(P^{\dagger}\right)_{n}**P_{n}**(-2)**\delta_{m,n1}**\left(P^{\dagger}\right)_{m}**P_{m}**\left(P^{\dagger}\right)_{n2}**\left(P^{\dagger}\right)_{n3}\,\mathrm{dyn}_{n,m}\,\delta_{n,m}\,c_{n1,n2,n3}$$

```
lhs8 = lhs7 //. clean
```

$$\frac{1}{2} (P^\dagger)_n ** (P^\dagger)_m ** P_n ** (P^\dagger)_{n1} ** P_m ** (P^\dagger)_{n2} ** (P^\dagger)_{n3}\, \text{dyn}_{n,m}\, c_{n1,n2,n3} +$$
$$(P^\dagger)_n ** (P^\dagger)_{n1} ** (P^\dagger)_{n2} ** P_m ** (P^\dagger)_{n3}\, \text{jex}_{n,m}\, c_{n1,n2,n3} +$$
$$\frac{1}{2} (P^\dagger)_n ** (P^\dagger)_m ** P_n ** (P^\dagger)_{n2} ** (P^\dagger)_{n3}\, \text{dyn}_{n,m}\, \delta_{m,n1}\, c_{n1,n2,n3} -$$
$$(P^\dagger)_n ** (P^\dagger)_m ** P_n ** (P^\dagger)_m ** P_m ** (P^\dagger)_{n2} ** (P^\dagger)_{n3}\, \text{dyn}_{n,m}\, \delta_{m,n1}\, c_{n1,n2,n3} +$$
$$(P^\dagger)_n ** (P^\dagger)_{n2} ** (P^\dagger)_{n3}\, \text{jex}_{n,m}\, \delta_{m,n1}\, c_{n1,n2,n3} -$$
$$2 (P^\dagger)_n ** (P^\dagger)_m ** (P^\dagger)_{n2} ** P_m ** (P^\dagger)_{n3}\, \text{jex}_{n,m}\, \delta_{m,n1}\, c_{n1,n2,n3} +$$
$$(P^\dagger)_n ** (P^\dagger)_{n1} ** (P^\dagger)_{n3}\, \text{jex}_{n,m}\, \delta_{m,n2}\, c_{n1,n2,n3} -$$
$$2 (P^\dagger)_n ** (P^\dagger)_{n1} ** (P^\dagger)_m ** P_m ** (P^\dagger)_{n3}\, \text{jex}_{n,m}\, \delta_{m,n2}\, c_{n1,n2,n3} -$$
$$2 (P^\dagger)_n ** (P^\dagger)_m ** (P^\dagger)_{n3}\, \text{jex}_{n,m}\, \delta_{m,n1}\, \delta_{m,n2}\, c_{n1,n2,n3} +$$
$$4 (P^\dagger)_n ** (P^\dagger)_m ** (P^\dagger)_m ** P_m ** (P^\dagger)_{n3}\, \text{jex}_{n,m}\, \delta_{m,n1}\, \delta_{m,n2}\, c_{n1,n2,n3} +$$
$$\frac{1}{2} (P^\dagger)_n ** (P^\dagger)_{n1} ** P_m ** (P^\dagger)_{n2} ** (P^\dagger)_{n3}\, \text{dyn}_{n,m}\, \delta_{n,m}\, c_{n1,n2,n3} -$$
$$(P^\dagger)_n ** (P^\dagger)_n ** P_n ** (P^\dagger)_{n1} ** P_m ** (P^\dagger)_{n2} ** (P^\dagger)_{n3}\, \text{dyn}_{n,m}\, \delta_{n,m}\, c_{n1,n2,n3} +$$
$$\frac{1}{2} (P^\dagger)_n ** (P^\dagger)_{n2} ** (P^\dagger)_{n3}\, \text{dyn}_{n,m}\, \delta_{m,n1}\, \delta_{n,m}\, c_{n1,n2,n3} -$$
$$(P^\dagger)_n ** (P^\dagger)_m ** P_m ** (P^\dagger)_{n2} ** (P^\dagger)_{n3}\, \text{dyn}_{n,m}\, \delta_{m,n1}\, \delta_{n,m}\, c_{n1,n2,n3} -$$
$$(P^\dagger)_n ** (P^\dagger)_n ** P_n ** (P^\dagger)_{n2} ** (P^\dagger)_{n3}\, \text{dyn}_{n,m}\, \delta_{m,n1}\, \delta_{n,m}\, c_{n1,n2,n3} +$$
$$2 (P^\dagger)_n ** (P^\dagger)_n ** P_n ** (P^\dagger)_m ** P_m ** (P^\dagger)_{n2} ** (P^\dagger)_{n3}\, \text{dyn}_{n,m}\, \delta_{m,n1}\, \delta_{n,m}\, c_{n1,n2,n3}$$

```
lhs9 = deleteZeroTerm[lhs8]
```

$$\frac{1}{2} (P^\dagger)_n ** (P^\dagger)_m ** P_n ** (P^\dagger)_{n1} ** P_m ** (P^\dagger)_{n2} ** (P^\dagger)_{n3}\, \text{dyn}_{n,m}\, c_{n1,n2,n3} +$$
$$(P^\dagger)_n ** (P^\dagger)_{n1} ** (P^\dagger)_{n2} ** P_m ** (P^\dagger)_{n3}\, \text{jex}_{n,m}\, c_{n1,n2,n3} +$$
$$\frac{1}{2} (P^\dagger)_n ** (P^\dagger)_m ** P_n ** (P^\dagger)_{n2} ** (P^\dagger)_{n3}\, \text{dyn}_{n,m}\, \delta_{m,n1}\, c_{n1,n2,n3} -$$
$$(P^\dagger)_n ** (P^\dagger)_m ** P_n ** (P^\dagger)_m ** P_m ** (P^\dagger)_{n2} ** (P^\dagger)_{n3}\, \text{dyn}_{n,m}\, \delta_{m,n1}\, c_{n1,n2,n3} +$$
$$(P^\dagger)_n ** (P^\dagger)_{n2} ** (P^\dagger)_{n3}\, \text{jex}_{n,m}\, \delta_{m,n1}\, c_{n1,n2,n3} -$$
$$2 (P^\dagger)_n ** (P^\dagger)_m ** (P^\dagger)_{n2} ** P_m ** (P^\dagger)_{n3}\, \text{jex}_{n,m}\, \delta_{m,n1}\, c_{n1,n2,n3} +$$
$$(P^\dagger)_n ** (P^\dagger)_{n1} ** (P^\dagger)_{n3}\, \text{jex}_{n,m}\, \delta_{m,n2}\, c_{n1,n2,n3} -$$
$$2 (P^\dagger)_n ** (P^\dagger)_{n1} ** (P^\dagger)_m ** P_m ** (P^\dagger)_{n3}\, \text{jex}_{n,m}\, \delta_{m,n2}\, c_{n1,n2,n3} -$$
$$2 (P^\dagger)_n ** (P^\dagger)_m ** (P^\dagger)_{n3}\, \text{jex}_{n,m}\, \delta_{m,n1}\, \delta_{m,n2}\, c_{n1,n2,n3} +$$
$$4 (P^\dagger)_n ** (P^\dagger)_m ** (P^\dagger)_m ** P_m ** (P^\dagger)_{n3}\, \text{jex}_{n,m}\, \delta_{m,n1}\, \delta_{m,n2}\, c_{n1,n2,n3} +$$
$$\frac{1}{2} (P^\dagger)_n ** (P^\dagger)_{n1} ** P_m ** (P^\dagger)_{n2} ** (P^\dagger)_{n3}\, \text{dyn}_{n,m}\, \delta_{n,m}\, c_{n1,n2,n3} -$$
$$(P^\dagger)_n ** (P^\dagger)_n ** P_n ** (P^\dagger)_{n1} ** P_m ** (P^\dagger)_{n2} ** (P^\dagger)_{n3}\, \text{dyn}_{n,m}\, \delta_{n,m}\, c_{n1,n2,n3} +$$
$$\frac{1}{2} (P^\dagger)_n ** (P^\dagger)_{n2} ** (P^\dagger)_{n3}\, \text{dyn}_{n,m}\, \delta_{m,n1}\, \delta_{n,m}\, c_{n1,n2,n3} -$$
$$(P^\dagger)_n ** (P^\dagger)_m ** P_m ** (P^\dagger)_{n2} ** (P^\dagger)_{n3}\, \text{dyn}_{n,m}\, \delta_{m,n1}\, \delta_{n,m}\, c_{n1,n2,n3} -$$
$$(P^\dagger)_n ** (P^\dagger)_n ** P_n ** (P^\dagger)_{n2} ** (P^\dagger)_{n3}\, \text{dyn}_{n,m}\, \delta_{m,n1}\, \delta_{n,m}\, c_{n1,n2,n3} +$$
$$2 (P^\dagger)_n ** (P^\dagger)_n ** P_n ** (P^\dagger)_m ** P_m ** (P^\dagger)_{n2} ** (P^\dagger)_{n3}\, \text{dyn}_{n,m}\, \delta_{m,n1}\, \delta_{n,m}\, c_{n1,n2,n3}$$

```
lhs10 = lhs9 //. commutationRule //. expand // ExpandAll;
```

```
lhs11 = lhs10 //. clean
```

$$\frac{1}{2} \left(P^{\dagger}\right)_{n} ** \left(P^{\dagger}\right)_{m} ** \left(P^{\dagger}\right)_{n1} ** P_{n} ** \left(P^{\dagger}\right)_{n2} ** P_{m} ** \left(P^{\dagger}\right)_{n3} \text{dyn}_{n,m} c_{n1,n2,n3} +$$

$$\left(P^{\dagger}\right)_{n} ** \left(P^{\dagger}\right)_{n1} ** \left(P^{\dagger}\right)_{n2} ** \left(P^{\dagger}\right)_{n3} ** P_{m} \text{jex}_{n,m} c_{n1,n2,n3} +$$

$$\frac{1}{2} \left(P^{\dagger}\right)_{n} ** \left(P^{\dagger}\right)_{m} ** \left(P^{\dagger}\right)_{n2} ** P_{n} ** \left(P^{\dagger}\right)_{n3} \text{dyn}_{n,m} \delta_{m,n1} c_{n1,n2,n3} -$$

$$\left(P^{\dagger}\right)_{n} ** \left(P^{\dagger}\right)_{m} ** \left(P^{\dagger}\right)_{m} ** P_{n} ** \left(P^{\dagger}\right)_{n2} ** P_{m} ** \left(P^{\dagger}\right)_{n3} \text{dyn}_{n,m} \delta_{m,n1} c_{n1,n2,n3} +$$

$$\left(P^{\dagger}\right)_{n} ** \left(P^{\dagger}\right)_{n2} ** \left(P^{\dagger}\right)_{n3} \text{jex}_{n,m} \delta_{m,n1} c_{n1,n2,n3} -$$

$$2 \left(P^{\dagger}\right)_{n} ** \left(P^{\dagger}\right)_{m} ** \left(P^{\dagger}\right)_{n2} ** \left(P^{\dagger}\right)_{n3} ** P_{m} \text{jex}_{n,m} \delta_{m,n1} c_{n1,n2,n3} +$$

$$\frac{1}{2} \left(P^{\dagger}\right)_{n} ** \left(P^{\dagger}\right)_{m} ** \left(P^{\dagger}\right)_{n1} ** P_{n} ** \left(P^{\dagger}\right)_{n3} \text{dyn}_{n,m} \delta_{m,n2} c_{n1,n2,n3} -$$

$$\left(P^{\dagger}\right)_{n} ** \left(P^{\dagger}\right)_{m} ** \left(P^{\dagger}\right)_{n1} ** P_{n} ** \left(P^{\dagger}\right)_{m} ** P_{m} ** \left(P^{\dagger}\right)_{n3} \text{dyn}_{n,m} \delta_{m,n2} c_{n1,n2,n3} +$$

$$\left(P^{\dagger}\right)_{n} ** \left(P^{\dagger}\right)_{n1} ** \left(P^{\dagger}\right)_{n3} \text{jex}_{n,m} \delta_{m,n2} c_{n1,n2,n3} -$$

$$2 \left(P^{\dagger}\right)_{n} ** \left(P^{\dagger}\right)_{n1} ** \left(P^{\dagger}\right)_{m} ** \left(P^{\dagger}\right)_{n3} ** P_{m} \text{jex}_{n,m} \delta_{m,n2} c_{n1,n2,n3} -$$

$$\left(P^{\dagger}\right)_{n} ** \left(P^{\dagger}\right)_{m} ** \left(P^{\dagger}\right)_{m} ** P_{n} ** \left(P^{\dagger}\right)_{n3} \text{dyn}_{n,m} \delta_{m,n1} \delta_{m,n2} c_{n1,n2,n3} +$$

$$2 \left(P^{\dagger}\right)_{n} ** \left(P^{\dagger}\right)_{m} ** \left(P^{\dagger}\right)_{m} ** P_{n} ** \left(P^{\dagger}\right)_{m} ** P_{m} ** \left(P^{\dagger}\right)_{n3} \text{dyn}_{n,m} \delta_{m,n1} \delta_{m,n2} c_{n1,n2,n3} -$$

$$2 \left(P^{\dagger}\right)_{n} ** \left(P^{\dagger}\right)_{m} ** \left(P^{\dagger}\right)_{n3} \text{jex}_{n,m} \delta_{m,n1} \delta_{m,n2} c_{n1,n2,n3} +$$

$$4 \left(P^{\dagger}\right)_{n} ** \left(P^{\dagger}\right)_{m} ** \left(P^{\dagger}\right)_{m} ** \left(P^{\dagger}\right)_{n3} ** P_{m} \text{jex}_{n,m} \delta_{m,n1} \delta_{m,n2} c_{n1,n2,n3} +$$

$$\left(P^{\dagger}\right)_{n} ** \left(P^{\dagger}\right)_{n1} ** \left(P^{\dagger}\right)_{n2} \text{jex}_{n,m} \delta_{m,n3} c_{n1,n2,n3} -$$

$$2 \left(P^{\dagger}\right)_{n} ** \left(P^{\dagger}\right)_{n1} ** \left(P^{\dagger}\right)_{n2} ** \left(P^{\dagger}\right)_{m} ** P_{m} \text{jex}_{n,m} \delta_{m,n3} c_{n1,n2,n3} -$$

$$2 \left(P^{\dagger}\right)_{n} ** \left(P^{\dagger}\right)_{m} ** \left(P^{\dagger}\right)_{n2} \text{jex}_{n,m} \delta_{m,n1} \delta_{m,n3} c_{n1,n2,n3} +$$

$$4 \left(P^{\dagger}\right)_{n} ** \left(P^{\dagger}\right)_{m} ** \left(P^{\dagger}\right)_{n2} ** \left(P^{\dagger}\right)_{m} ** P_{m} \text{jex}_{n,m} \delta_{m,n1} \delta_{m,n3} c_{n1,n2,n3} -$$

$$2 \left(P^{\dagger}\right)_{n} ** \left(P^{\dagger}\right)_{n1} ** \left(P^{\dagger}\right)_{m} \text{jex}_{n,m} \delta_{m,n2} \delta_{m,n3} c_{n1,n2,n3} +$$

$$4 \left(P^{\dagger}\right)_{n} ** \left(P^{\dagger}\right)_{n1} ** \left(P^{\dagger}\right)_{m} ** \left(P^{\dagger}\right)_{m} ** P_{m} \text{jex}_{n,m} \delta_{m,n2} \delta_{m,n3} c_{n1,n2,n3} +$$

$$4 \left(P^{\dagger}\right)_{n} ** \left(P^{\dagger}\right)_{m} ** \left(P^{\dagger}\right)_{m} \text{jex}_{n,m} \delta_{m,n1} \delta_{m,n2} \delta_{m,n3} c_{n1,n2,n3} -$$

$$8 \left(P^{\dagger}\right)_{n} ** \left(P^{\dagger}\right)_{m} ** \left(P^{\dagger}\right)_{m} ** \left(P^{\dagger}\right)_{m} ** P_{m} \text{jex}_{n,m} \delta_{m,n1} \delta_{m,n2} \delta_{m,n3} c_{n1,n2,n3} +$$

$$\frac{1}{2} \left(P^{\dagger}\right)_{n} ** \left(P^{\dagger}\right)_{n1} ** \left(P^{\dagger}\right)_{n2} ** P_{m} ** \left(P^{\dagger}\right)_{n3} \text{dyn}_{n,m} \delta_{n,m} c_{n1,n2,n3} -$$

$$\left(P^{\dagger}\right)_{n} ** \left(P^{\dagger}\right)_{n} ** \left(P^{\dagger}\right)_{n1} ** P_{n} ** \left(P^{\dagger}\right)_{n2} ** P_{m} ** \left(P^{\dagger}\right)_{n3} \text{dyn}_{n,m} \delta_{n,m} c_{n1,n2,n3} +$$

$$\frac{1}{2} \left(P^{\dagger}\right)_{n} ** \left(P^{\dagger}\right)_{n2} ** \left(P^{\dagger}\right)_{n3} \text{dyn}_{n,m} \delta_{m,n1} \delta_{n,m} c_{n1,n2,n3} -$$

$$2 \left(P^{\dagger}\right)_{n} ** \left(P^{\dagger}\right)_{m} ** \left(P^{\dagger}\right)_{n2} ** P_{m} ** \left(P^{\dagger}\right)_{n3} \text{dyn}_{n,m} \delta_{m,n1} \delta_{n,m} c_{n1,n2,n3} -$$

$$\left(P^{\dagger}\right)_{n} ** \left(P^{\dagger}\right)_{n} ** \left(P^{\dagger}\right)_{n2} ** P_{n} ** \left(P^{\dagger}\right)_{n3} \text{dyn}_{n,m} \delta_{m,n1} \delta_{n,m} c_{n1,n2,n3} +$$

$$2 \left(P^{\dagger}\right)_{n} ** \left(P^{\dagger}\right)_{m} ** \left(P^{\dagger}\right)_{n} ** P_{n} ** \left(P^{\dagger}\right)_{n2} ** P_{m} ** \left(P^{\dagger}\right)_{n3} \text{dyn}_{n,m} \delta_{m,n1} \delta_{n,m} c_{n1,n2,n3} +$$

$$2 \left(P^{\dagger}\right)_{n} ** \left(P^{\dagger}\right)_{n} ** \left(P^{\dagger}\right)_{m} ** P_{n} ** \left(P^{\dagger}\right)_{n2} ** P_{m} ** \left(P^{\dagger}\right)_{n3} \text{dyn}_{n,m} \delta_{m,n1} \delta_{n,m} c_{n1,n2,n3} +$$

$$\frac{1}{2} \left(P^{\dagger}\right)_{n} ** \left(P^{\dagger}\right)_{n1} ** \left(P^{\dagger}\right)_{n3} \text{dyn}_{n,m} \delta_{m,n2} \delta_{n,m} c_{n1,n2,n3} -$$

$$\left(P^{\dagger}\right)_{n} ** \left(P^{\dagger}\right)_{n} ** \left(P^{\dagger}\right)_{n1} ** P_{n} ** \left(P^{\dagger}\right)_{n3} \text{dyn}_{n,m} \delta_{m,n2} \delta_{n,m} c_{n1,n2,n3} -$$

$$\left(P^{\dagger}\right)_{n} ** \left(P^{\dagger}\right)_{n1} ** \left(P^{\dagger}\right)_{m} ** P_{m} ** \left(P^{\dagger}\right)_{n3} \text{dyn}_{n,m} \delta_{m,n2} \delta_{n,m} c_{n1,n2,n3} +$$

$2\,(P^\dagger)_n ** (P^\dagger)_n ** (P^\dagger)_{n1} ** P_n ** (P^\dagger)_m ** P_m ** (P^\dagger)_{n3}\, dyn_{n,m}\, \delta_{m,n2}\, \delta_{n,m}\, c_{n1,n2,n3} -$
$2\,(P^\dagger)_n ** (P^\dagger)_m ** (P^\dagger)_{n3}\, dyn_{n,m}\, \delta_{m,n1}\, \delta_{m,n2}\, \delta_{n,m}\, c_{n1,n2,n3} +$
$4\,(P^\dagger)_n ** (P^\dagger)_m ** (P^\dagger)_m ** P_m ** (P^\dagger)_{n3}\, dyn_{n,m}\, \delta_{m,n1}\, \delta_{m,n2}\, \delta_{n,m}\, c_{n1,n2,n3} +$
$2\,(P^\dagger)_n ** (P^\dagger)_m ** (P^\dagger)_n ** P_n ** (P^\dagger)_{n3}\, dyn_{n,m}\, \delta_{m,n1}\, \delta_{m,n2}\, \delta_{n,m}\, c_{n1,n2,n3} +$
$2\,(P^\dagger)_n ** (P^\dagger)_n ** (P^\dagger)_m ** P_n ** (P^\dagger)_{n3}\, dyn_{n,m}\, \delta_{m,n1}\, \delta_{m,n2}\, \delta_{n,m}\, c_{n1,n2,n3} -$
$4\,(P^\dagger)_n ** (P^\dagger)_m ** (P^\dagger)_n ** P_n ** (P^\dagger)_m ** P_m ** (P^\dagger)_{n3}\, dyn_{n,m}\, \delta_{m,n1}\, \delta_{m,n2}\, \delta_{n,m}\, c_{n1,n2,n3} -$
$4\,(P^\dagger)_n ** (P^\dagger)_n ** (P^\dagger)_m ** P_n ** (P^\dagger)_m ** P_m ** (P^\dagger)_{n3}\, dyn_{n,m}\, \delta_{m,n1}\, \delta_{m,n2}\, \delta_{n,m}\, c_{n1,n2,n3} +$
$2\,(P^\dagger)_n ** (P^\dagger)_n ** (P^\dagger)_{n2} ** P_m ** (P^\dagger)_{n3}\, dyn_{n,m}\, \delta_{m,n1}\, \delta_{n,m}^2\, c_{n1,n2,n3} -$
$4\,(P^\dagger)_n ** (P^\dagger)_n ** (P^\dagger)_n ** P_n ** (P^\dagger)_{n2} ** P_m ** (P^\dagger)_{n3}\, dyn_{n,m}\, \delta_{m,n1}\, \delta_{n,m}^2\, c_{n1,n2,n3} +$
$2\,(P^\dagger)_n ** (P^\dagger)_n ** (P^\dagger)_{n3}\, dyn_{n,m}\, \delta_{m,n1}\, \delta_{m,n2}\, \delta_{n,m}^2\, c_{n1,n2,n3} -$
$4\,(P^\dagger)_n ** (P^\dagger)_n ** (P^\dagger)_m ** P_m ** (P^\dagger)_{n3}\, dyn_{n,m}\, \delta_{m,n1}\, \delta_{m,n2}\, \delta_{n,m}^2\, c_{n1,n2,n3} -$
$4\,(P^\dagger)_n ** (P^\dagger)_n ** (P^\dagger)_n ** P_n ** (P^\dagger)_{n3}\, dyn_{n,m}\, \delta_{m,n1}\, \delta_{m,n2}\, \delta_{n,m}^2\, c_{n1,n2,n3} +$
$8\,(P^\dagger)_n ** (P^\dagger)_n ** (P^\dagger)_n ** P_n ** (P^\dagger)_m ** P_m ** (P^\dagger)_{n3}\, dyn_{n,m}\, \delta_{m,n1}\, \delta_{m,n2}\, \delta_{n,m}^2\, c_{n1,n2,n3} +$
$\frac{1}{2}\,(P^\dagger)_n ** (P^\dagger)_m ** (P^\dagger)_{n2} ** P_m ** (P^\dagger)_{n3}\, dyn_{n,m}\, \delta_{n,n1}\, c_{n1,n2,n3} -$
$(P^\dagger)_n ** (P^\dagger)_m ** (P^\dagger)_n ** P_n ** (P^\dagger)_{n2} ** P_m ** (P^\dagger)_{n3}\, dyn_{n,m}\, \delta_{n,n1}\, c_{n1,n2,n3} +$
$\frac{1}{2}\,(P^\dagger)_n ** (P^\dagger)_m ** (P^\dagger)_{n3}\, dyn_{n,m}\, \delta_{m,n2}\, \delta_{n,n1}\, c_{n1,n2,n3} -$
$(P^\dagger)_n ** (P^\dagger)_m ** (P^\dagger)_m ** P_m ** (P^\dagger)_{n3}\, dyn_{n,m}\, \delta_{m,n2}\, \delta_{n,n1}\, c_{n1,n2,n3} -$
$(P^\dagger)_n ** (P^\dagger)_m ** (P^\dagger)_n ** P_n ** (P^\dagger)_{n3}\, dyn_{n,m}\, \delta_{m,n2}\, \delta_{n,n1}\, c_{n1,n2,n3} +$
$2\,(P^\dagger)_n ** (P^\dagger)_m ** (P^\dagger)_n ** P_n ** (P^\dagger)_m ** P_m ** (P^\dagger)_{n3}\, dyn_{n,m}\, \delta_{m,n2}\, \delta_{n,n1}\, c_{n1,n2,n3} -$
$(P^\dagger)_n ** (P^\dagger)_n ** (P^\dagger)_{n2} ** P_m ** (P^\dagger)_{n3}\, dyn_{n,m}\, \delta_{n,m}\, \delta_{n,n1}\, c_{n1,n2,n3} +$
$2\,(P^\dagger)_n ** (P^\dagger)_n ** (P^\dagger)_n ** P_n ** (P^\dagger)_{n2} ** P_m ** (P^\dagger)_{n3}\, dyn_{n,m}\, \delta_{n,m}\, \delta_{n,n1}\, c_{n1,n2,n3} -$
$(P^\dagger)_n ** (P^\dagger)_n ** (P^\dagger)_{n3}\, dyn_{n,m}\, \delta_{m,n2}\, \delta_{n,m}\, \delta_{n,n1}\, c_{n1,n2,n3} +$
$2\,(P^\dagger)_n ** (P^\dagger)_n ** (P^\dagger)_m ** P_m ** (P^\dagger)_{n3}\, dyn_{n,m}\, \delta_{m,n2}\, \delta_{n,m}\, \delta_{n,n1}\, c_{n1,n2,n3} +$
$2\,(P^\dagger)_n ** (P^\dagger)_n ** (P^\dagger)_n ** P_n ** (P^\dagger)_{n3}\, dyn_{n,m}\, \delta_{m,n2}\, \delta_{n,m}\, \delta_{n,n1}\, c_{n1,n2,n3} -$
$4\,(P^\dagger)_n ** (P^\dagger)_n ** (P^\dagger)_n ** P_n ** (P^\dagger)_m ** P_m ** (P^\dagger)_{n3}\, dyn_{n,m}\, \delta_{m,n2}\, \delta_{n,m}\, \delta_{n,n1}\, c_{n1,n2,n3} +$
$\frac{1}{2}\,(P^\dagger)_n ** (P^\dagger)_m ** (P^\dagger)_{n3}\, dyn_{n,m}\, \delta_{m,n1}\, \delta_{n,n2}\, c_{n1,n2,n3} -$
$(P^\dagger)_n ** (P^\dagger)_m ** (P^\dagger)_n ** P_n ** (P^\dagger)_{n3}\, dyn_{n,m}\, \delta_{m,n1}\, \delta_{n,n2}\, c_{n1,n2,n3} -$
$(P^\dagger)_n ** (P^\dagger)_n ** (P^\dagger)_{n3}\, dyn_{n,m}\, \delta_{m,n1}\, \delta_{n,m}\, \delta_{n,n2}\, c_{n1,n2,n3} +$
$2\,(P^\dagger)_n ** (P^\dagger)_n ** (P^\dagger)_n ** P_n ** (P^\dagger)_{n3}\, dyn_{n,m}\, \delta_{m,n1}\, \delta_{n,m}\, \delta_{n,n2}\, c_{n1,n2,n3}$

lhs12 = deleteZeroTerm[lhs11] /. $\{\delta_{n,m} \to 0,\ \delta_{m,n} \to 0\}$
(* We want to get rid of the terms that contain $\delta_{m,n}$ and $\delta_{n,m}$ because they will make $dyn_{n,m}$ and $jex_{n,m}$ becomes $dyn_{n,n}$ and $jex_{n,n}$ which are zero. Note all terms will appear within the summation over n and m. *)

$$\frac{1}{2}\left(P^{\dagger}\right)_{n} ** \left(P^{\dagger}\right)_{m} ** \left(P^{\dagger}\right)_{n1} ** P_{n} ** \left(P^{\dagger}\right)_{n2} ** P_{m} ** \left(P^{\dagger}\right)_{n3}\, \mathrm{dyn}_{n,m}\, c_{n1,n2,n3} +$$

$$\frac{1}{2}\left(P^{\dagger}\right)_{n} ** \left(P^{\dagger}\right)_{m} ** \left(P^{\dagger}\right)_{n2} ** P_{n} ** \left(P^{\dagger}\right)_{n3}\, \mathrm{dyn}_{n,m}\, \delta_{m,n1}\, c_{n1,n2,n3} -$$

$$\left(P^{\dagger}\right)_{n} ** \left(P^{\dagger}\right)_{m} ** \left(P^{\dagger}\right)_{m} ** P_{n} ** \left(P^{\dagger}\right)_{n2} ** P_{m} ** \left(P^{\dagger}\right)_{n3}\, \mathrm{dyn}_{n,m}\, \delta_{m,n1}\, c_{n1,n2,n3} +$$

$$\left(P^{\dagger}\right)_{n} ** \left(P^{\dagger}\right)_{n2} ** \left(P^{\dagger}\right)_{n3}\, \mathrm{jex}_{n,m}\, \delta_{m,n1}\, c_{n1,n2,n3} +$$

$$\frac{1}{2}\left(P^{\dagger}\right)_{n} ** \left(P^{\dagger}\right)_{m} ** \left(P^{\dagger}\right)_{n1} ** P_{n} ** \left(P^{\dagger}\right)_{n3}\, \mathrm{dyn}_{n,m}\, \delta_{m,n2}\, c_{n1,n2,n3} -$$

$$\left(P^{\dagger}\right)_{n} ** \left(P^{\dagger}\right)_{m} ** \left(P^{\dagger}\right)_{n1} ** P_{n} ** \left(P^{\dagger}\right)_{m} ** P_{m} ** \left(P^{\dagger}\right)_{n3}\, \mathrm{dyn}_{n,m}\, \delta_{m,n2}\, c_{n1,n2,n3} +$$

$$\left(P^{\dagger}\right)_{n} ** \left(P^{\dagger}\right)_{n1} ** \left(P^{\dagger}\right)_{n3}\, \mathrm{jex}_{n,m}\, \delta_{m,n2}\, c_{n1,n2,n3} -$$

$$\left(P^{\dagger}\right)_{n} ** \left(P^{\dagger}\right)_{m} ** \left(P^{\dagger}\right)_{m} ** P_{n} ** \left(P^{\dagger}\right)_{n3}\, \mathrm{dyn}_{n,m}\, \delta_{m,n1}\, \delta_{m,n2}\, c_{n1,n2,n3} +$$

$$2\left(P^{\dagger}\right)_{n} ** \left(P^{\dagger}\right)_{m} ** \left(P^{\dagger}\right)_{m} ** P_{n} ** \left(P^{\dagger}\right)_{m} ** P_{m} ** \left(P^{\dagger}\right)_{n3}\, \mathrm{dyn}_{n,m}\, \delta_{m,n1}\, \delta_{m,n2}\, c_{n1,n2,n3} -$$

$$2\left(P^{\dagger}\right)_{n} ** \left(P^{\dagger}\right)_{m} ** \left(P^{\dagger}\right)_{n3}\, \mathrm{jex}_{n,m}\, \delta_{m,n1}\, \delta_{m,n2}\, c_{n1,n2,n3} +$$

$$\left(P^{\dagger}\right)_{n} ** \left(P^{\dagger}\right)_{n1} ** \left(P^{\dagger}\right)_{n2}\, \mathrm{jex}_{n,m}\, \delta_{m,n3}\, c_{n1,n2,n3} - 2\left(P^{\dagger}\right)_{n} ** \left(P^{\dagger}\right)_{m} ** \left(P^{\dagger}\right)_{n2}\, \mathrm{jex}_{n,m}\, \delta_{m,n1}\, \delta_{m,n3}\, c_{n1,n2,n3} -$$

$$2\left(P^{\dagger}\right)_{n} ** \left(P^{\dagger}\right)_{n1} ** \left(P^{\dagger}\right)_{m}\, \mathrm{jex}_{n,m}\, \delta_{m,n2}\, \delta_{m,n3}\, c_{n1,n2,n3} +$$

$$4\left(P^{\dagger}\right)_{n} ** \left(P^{\dagger}\right)_{m} ** \left(P^{\dagger}\right)_{m}\, \mathrm{jex}_{n,m}\, \delta_{m,n1}\, \delta_{m,n2}\, \delta_{m,n3}\, c_{n1,n2,n3} +$$

$$\frac{1}{2}\left(P^{\dagger}\right)_{n} ** \left(P^{\dagger}\right)_{m} ** \left(P^{\dagger}\right)_{n2} ** P_{m} ** \left(P^{\dagger}\right)_{n3}\, \mathrm{dyn}_{n,m}\, \delta_{n,n1}\, c_{n1,n2,n3} -$$

$$\left(P^{\dagger}\right)_{n} ** \left(P^{\dagger}\right)_{m} ** \left(P^{\dagger}\right)_{n} ** P_{n} ** \left(P^{\dagger}\right)_{n2} ** P_{m} ** \left(P^{\dagger}\right)_{n3}\, \mathrm{dyn}_{n,m}\, \delta_{n,n1}\, c_{n1,n2,n3} +$$

$$\frac{1}{2}\left(P^{\dagger}\right)_{n} ** \left(P^{\dagger}\right)_{m} ** \left(P^{\dagger}\right)_{n3}\, \mathrm{dyn}_{n,m}\, \delta_{m,n2}\, \delta_{n,n1}\, c_{n1,n2,n3} -$$

$$\left(P^{\dagger}\right)_{n} ** \left(P^{\dagger}\right)_{m} ** \left(P^{\dagger}\right)_{m} ** P_{m} ** \left(P^{\dagger}\right)_{n3}\, \mathrm{dyn}_{n,m}\, \delta_{m,n2}\, \delta_{n,n1}\, c_{n1,n2,n3} -$$

$$\left(P^{\dagger}\right)_{n} ** \left(P^{\dagger}\right)_{m} ** \left(P^{\dagger}\right)_{n} ** P_{n} ** \left(P^{\dagger}\right)_{n3}\, \mathrm{dyn}_{n,m}\, \delta_{m,n2}\, \delta_{n,n1}\, c_{n1,n2,n3} +$$

$$2\left(P^{\dagger}\right)_{n} ** \left(P^{\dagger}\right)_{m} ** \left(P^{\dagger}\right)_{n} ** P_{n} ** \left(P^{\dagger}\right)_{m} ** P_{m} ** \left(P^{\dagger}\right)_{n3}\, \mathrm{dyn}_{n,m}\, \delta_{m,n2}\, \delta_{n,n1}\, c_{n1,n2,n3} +$$

$$\frac{1}{2}\left(P^{\dagger}\right)_{n} ** \left(P^{\dagger}\right)_{m} ** \left(P^{\dagger}\right)_{n3}\, \mathrm{dyn}_{n,m}\, \delta_{m,n1}\, \delta_{n,n2}\, c_{n1,n2,n3} -$$

$$\left(P^{\dagger}\right)_{n} ** \left(P^{\dagger}\right)_{m} ** \left(P^{\dagger}\right)_{n} ** P_{n} ** \left(P^{\dagger}\right)_{n3}\, \mathrm{dyn}_{n,m}\, \delta_{m,n1}\, \delta_{n,n2}\, c_{n1,n2,n3}$$

```
lhs13 = lhs12 //. commutationRule //. expand // ExpandAll;
lhs14 = lhs13 //. clean;
Length[lhs14]
lhs15 = deleteZeroTerm[lhs14] /. {δn,m → 0, δm,n → 0}
Length[lhs15]
```

84

$$\begin{aligned}&(P^\dagger)_n ** (P^\dagger)_{n2} ** (P^\dagger)_{n3}\, jex_{n,m}\, \delta_{m,n1}\, c_{n1,n2,n3} + \\
&(P^\dagger)_n ** (P^\dagger)_{n1} ** (P^\dagger)_{n3}\, jex_{n,m}\, \delta_{m,n2}\, c_{n1,n2,n3} - 2\,(P^\dagger)_n ** (P^\dagger)_m ** (P^\dagger)_{n3}\, jex_{n,m}\, \delta_{m,n1}\,\delta_{m,n2}\, c_{n1,n2,n3} + \\
&(P^\dagger)_n ** (P^\dagger)_{n1} ** (P^\dagger)_{n2}\, jex_{n,m}\, \delta_{m,n3}\, c_{n1,n2,n3} - 2\,(P^\dagger)_n ** (P^\dagger)_m ** (P^\dagger)_{n2}\, jex_{n,m}\, \delta_{m,n1}\,\delta_{m,n3}\, c_{n1,n2,n3} - \\
&2\,(P^\dagger)_n ** (P^\dagger)_{n1} ** (P^\dagger)_m\, jex_{n,m}\, \delta_{m,n2}\,\delta_{m,n3}\, c_{n1,n2,n3} + \\
&4\,(P^\dagger)_n ** (P^\dagger)_m ** (P^\dagger)_m\, jex_{n,m}\, \delta_{m,n1}\,\delta_{m,n2}\,\delta_{m,n3}\, c_{n1,n2,n3} + \\
&\frac{1}{2}\,(P^\dagger)_n ** (P^\dagger)_m ** (P^\dagger)_{n3}\, dyn_{n,m}\, \delta_{m,n2}\,\delta_{n,n1}\, c_{n1,n2,n3} + \\
&\frac{1}{2}\,(P^\dagger)_n ** (P^\dagger)_m ** (P^\dagger)_{n2}\, dyn_{n,m}\, \delta_{m,n3}\,\delta_{n,n1}\, c_{n1,n2,n3} - \\
&(P^\dagger)_n ** (P^\dagger)_m ** (P^\dagger)_m\, dyn_{n,m}\, \delta_{m,n2}\,\delta_{m,n3}\,\delta_{n,n1}\, c_{n1,n2,n3} + \\
&\frac{1}{2}\,(P^\dagger)_n ** (P^\dagger)_m ** (P^\dagger)_{n3}\, dyn_{n,m}\, \delta_{m,n1}\,\delta_{n,n2}\, c_{n1,n2,n3} + \\
&\frac{1}{2}\,(P^\dagger)_n ** (P^\dagger)_m ** (P^\dagger)_{n1}\, dyn_{n,m}\, \delta_{m,n3}\,\delta_{n,n2}\, c_{n1,n2,n3} - \\
&(P^\dagger)_n ** (P^\dagger)_m ** (P^\dagger)_m\, dyn_{n,m}\, \delta_{m,n1}\,\delta_{m,n3}\,\delta_{n,n2}\, c_{n1,n2,n3} - \\
&(P^\dagger)_n ** (P^\dagger)_m ** (P^\dagger)_n\, dyn_{n,m}\, \delta_{m,n3}\,\delta_{n,n1}\,\delta_{n,n2}\, c_{n1,n2,n3} + \\
&\frac{1}{2}\,(P^\dagger)_n ** (P^\dagger)_m ** (P^\dagger)_{n2}\, dyn_{n,m}\, \delta_{m,n1}\,\delta_{n,n3}\, c_{n1,n2,n3} + \\
&\frac{1}{2}\,(P^\dagger)_n ** (P^\dagger)_m ** (P^\dagger)_{n1}\, dyn_{n,m}\, \delta_{m,n2}\,\delta_{n,n3}\, c_{n1,n2,n3} - \\
&(P^\dagger)_n ** (P^\dagger)_m ** (P^\dagger)_m\, dyn_{n,m}\, \delta_{m,n1}\,\delta_{m,n2}\,\delta_{n,n3}\, c_{n1,n2,n3} - \\
&(P^\dagger)_n ** (P^\dagger)_m ** (P^\dagger)_n\, dyn_{n,m}\, \delta_{m,n2}\,\delta_{n,n1}\,\delta_{n,n3}\, c_{n1,n2,n3} - \\
&(P^\dagger)_n ** (P^\dagger)_m ** (P^\dagger)_n\, dyn_{n,m}\, \delta_{m,n1}\,\delta_{n,n2}\,\delta_{n,n3}\, c_{n1,n2,n3}\end{aligned}$$

19

Note that the terms which contain $\delta_{n,n2}\,\delta_{n,n3}$ and $\delta_{n,n2}\,\delta_{n,n3}\delta_{n,n3}$ will be zero

```
lhs16 = lhs15 /. {δn,n2_ δn,n3_ → 0, δm,n2_ δm,n3_ → 0, δn,n1_ δn,n2_ δn,n3_ → 0, δm,n1_ δm,n2_ δm,n3_ → 0}
```

$$\begin{aligned}&(P^\dagger)_n ** (P^\dagger)_{n2} ** (P^\dagger)_{n3}\, jex_{n,m}\, \delta_{m,n1}\, c_{n1,n2,n3} + (P^\dagger)_n ** (P^\dagger)_{n1} ** (P^\dagger)_{n3}\, jex_{n,m}\, \delta_{m,n2}\, c_{n1,n2,n3} + \\
&(P^\dagger)_n ** (P^\dagger)_{n1} ** (P^\dagger)_{n2}\, jex_{n,m}\, \delta_{m,n3}\, c_{n1,n2,n3} + \frac{1}{2}\,(P^\dagger)_n ** (P^\dagger)_m ** (P^\dagger)_{n3}\, dyn_{n,m}\, \delta_{m,n2}\,\delta_{n,n1}\, c_{n1,n2,n3} + \\
&\frac{1}{2}\,(P^\dagger)_n ** (P^\dagger)_m ** (P^\dagger)_{n2}\, dyn_{n,m}\, \delta_{m,n3}\,\delta_{n,n1}\, c_{n1,n2,n3} + \\
&\frac{1}{2}\,(P^\dagger)_n ** (P^\dagger)_m ** (P^\dagger)_{n3}\, dyn_{n,m}\, \delta_{m,n1}\,\delta_{n,n2}\, c_{n1,n2,n3} + \\
&\frac{1}{2}\,(P^\dagger)_n ** (P^\dagger)_m ** (P^\dagger)_{n1}\, dyn_{n,m}\, \delta_{m,n3}\,\delta_{n,n2}\, c_{n1,n2,n3} + \\
&\frac{1}{2}\,(P^\dagger)_n ** (P^\dagger)_m ** (P^\dagger)_{n2}\, dyn_{n,m}\, \delta_{m,n1}\,\delta_{n,n3}\, c_{n1,n2,n3} + \\
&\frac{1}{2}\,(P^\dagger)_n ** (P^\dagger)_m ** (P^\dagger)_{n1}\, dyn_{n,m}\, \delta_{m,n2}\,\delta_{n,n3}\, c_{n1,n2,n3}\end{aligned}$$

The first three terms are equivalent to (exchanging index n1 and n, ...)

$$\sum_{n1,n2,n3}\sum_m\sum_n (P^\dagger)_n ** (P^\dagger)_{n2} ** (P^\dagger)_{n3}\, jex_{n,m}\, \delta_{m,n1}\, c_{n1,n2,n3} + (P^\dagger)_n ** (P^\dagger)_{n1} ** (P^\dagger)_{n3}\, jex_{n,m}\, \delta_{m,n2}\, c_{n1,n2,n3} + (P^\dagger)_n ** (P^\dagger)_{n1} ** (P^\dagger)_{n2}\, jex_{n,m}\, \delta_{m,n3}\, c_{n1,n2,n3}$$

$$= \sum_{n1,n2,n3}\sum_n (P^\dagger)_n ** (P^\dagger)_{n2} ** (P^\dagger)_{n3}\, J(n, n1)\, c_{n1,n2,n3} + (P^\dagger)_n ** (P^\dagger)_{n1} ** (P^\dagger)_{n3}\, J(n, n2)\, c_{n1,n2,n3} + (P^\dagger)_n ** (P^\dagger)_{n1} ** (P^\dagger)_{n2}\, J(n, n3)\, c_{n1,n2,n3}$$

$$= \sum_{n1,n2,n3}\sum_n (P^\dagger)_{n1} ** (P^\dagger)_{n2} ** (P^\dagger)_{n3}\, J(n, n1)\, c_{n,n2,n3} + (P^\dagger)_{n1} ** (P^\dagger)_{n2} ** (P^\dagger)_{n3}\, J(n, n2)\, c_{n1,n,n3} + (P^\dagger)_{n1} ** (P^\dagger)_{n2} ** (P^\dagger)_{n3}\, J(n, n3)\, c_{n1,n2,n}$$

The last six terms are equivalent to

$$\sum_{n1,n2,n3}\sum_m\sum_n (P^\dagger)_n ** (P^\dagger)_m ** (P^\dagger)_{n3}\, dyn_{n,m}\, \delta_{m,n2}\, \delta_{n,n1}\, c_{n1,n2,n3} + (P^\dagger)_n ** (P^\dagger)_m ** (P^\dagger)_{n2}\, dyn_{n,m}\, \delta_{m,n3}\, \delta_{n,n1}\, c_{n1,n2,n3} + (P^\dagger)_n ** (P^\dagger)_m ** (P^\dagger)_{n1}\, dyn_{n,m}\, \delta_{m,n3}\, \delta_{n,n2}\, c_{n1,n2,n3}$$

$$= \sum_{n1,n2,n3} (P^\dagger)_n ** (P^\dagger)_m ** (P^\dagger)_{n3}\; c_{n1,n2,n3}\,[D(n1-n2) + D(n1-n3) + D(n2-n3)]$$

Therefore, the lhs16 term is equivalent to

$$\sum_{n1,n2,n3} (P^\dagger)_n ** (P^\dagger)_m ** (P^\dagger)_{n3} \times \Big\{ c_{n1,n2,n3}[D(n1-n2) + D(n1-n3) + D(n2-n3)] + \sum_n \big[J(n, n1)\, c_{n,n2,n3} + J(n, n2)\, c_{n1,n,n3} + J(n, n3)\, c_{n1,n2,n}\big]\Big\}$$

Adding up lhs0,

we can obtan the whole left - hand side of the Schroding equation

$$\sum_{n1,n2,n3} (P^\dagger)_n ** (P^\dagger)_m ** (P^\dagger)_{n3} \times \Big\{ c_{n1,n2,n3}[D(n1-n2) + D(n1-n3) + D(n2-n3)] + \sum_n \big[J(n, n1)\, c_{n,n2,n3} + J(n, n2)\, c_{n1,n,n3} + J(n, n3)\, c_{n1,n2,n}\big]\Big\} + \sum_{n1,n2,n3} (P^\dagger)_n ** (P^\dagger)_m ** (P^\dagger)_{n3}\, 3\,\epsilon_0\, c_{n1,n2,n3}$$

$$= \sum_{n1,n2,n3} (P^\dagger)_n ** (P^\dagger)_m ** (P^\dagger)_{n3}\, \epsilon\, c_{n1,n2,n3}$$

This leads to

$$(3\,\epsilon_0 - \epsilon)\, c_{n1,n2,n3} + \sum_n \left[J\,(n,\; n1)\, c_{n,\,n2,\,n3} + J\,(n - n2)\, c_{n1,\,n,\,n3} + J\,(n - n3)\, c_{n1,\,n2,\,n}\right] + c_{n1,n2,n3}\,[\,D\,(n1 - n2) + D\,(n1 - n3) + D\,(n2 - n3)\,] = 0$$

The above equation is defined only for the cases where $n1 \neq n2 \neq n3$. In order to make the left - hand side of it equivalent to the case of three noninteracting bosons, we add certain terms to the right - hand side of the equation

$$(3\,\epsilon_0 - \epsilon)\, c_{n1,n2,n3} + \sum_n \left[J\,(n - n1)\, c_{n,\,n2,\,n3} + J\,(n - n2)\, c_{n1,\,n,\,n3} + J\,(n,\; n3)\, c_{n1,\,n2,\,n}\right] + c_{n1,n2,n3}\,[\,D\,(n1 - n2) + D\,(n1 - n3) + D\,(n2 - n3)\,]$$

$$= 2\,\delta_{n1,n2} \sum_n J\,(n1 - n)\, c_{n,\,n2,\,n3} + 2\,\delta_{n2,n3} \sum_n J\,(n2 - n)\, c_{n1,\,n,\,n3} + 2\,\delta_{n1,n3} \sum_n J\,(n3 - n)\, c_{n1,\,n2,\,n}$$

It is easy to verify the above equation is hold (assumming that $c_{n1,n2,n3}$ is zero if any two of n1, n2, n3 are equal)

Now the Schrodinger equation has been reduced in site representation. In the next step, we will convert it into wave vector representation

At this point, it is better to work with the derivations by hand. We consider the above Schrodinger - like equation (including kinematic interaction) term by term.

Making use of the Fourier transform:

$$c_{n1,\,n2,\,n3} = \sum_{k1,\,k2,\,k3} e^{i\,(k1\,n1 + k2\,n2 + k3\,n3)}\, c\,(k1,\, k2,\, k3)$$

and

$$\sum_n e^{ik\,(n-m)}\, J\,(n - m) = J\,(k)\quad (k \text{ is a wave vector})$$

and

$$\sum_n e^{ik\,(n-m)}\, D\,(n - m) = D\,(k)$$

and the orthonormality relation

$$\delta_{n,m} = \frac{1}{N} \sum_k e^{ik\,(n-m)}$$

we are ready to convert the equation term by term.

$$\sum_n J(n-n1)\, c_{n,\,n2,\,n3}$$

$$= \frac{1}{\left(\sqrt{N}\right)^3} \times \sum_n \sum_{k1,k2,k3} J(n-n1)\, e^{i\,(k1\,n + k2\,n2 + k3\,n3)}\, c(k1,\,k2,\,k3)$$

$$= \frac{1}{\left(\sqrt{N}\right)^3} \times \sum_n \sum_{k1,k2,k3} J(n-n1)\, e^{ik1\,(n-n1)}\, e^{i\,(k1\,n1 + k2\,n2 + k3\,n3)}\, c(k1,\,k2,\,k3)$$

$$= \frac{1}{\left(\sqrt{N}\right)^3} \sum_{k1,k2,k3} J(k1)\, e^{i\,(k1\,n1 + k2\,n2 + k3\,n3)}\, c(k1,\,k2,\,k3)$$

For the other two similar terms, we can do the similar things. Then

$$\sum_n \left[J(n-n1)\, c_{n,\,n2,\,n3} + J(n-n2)\, c_{n1,\,n,\,n3} + J(n,\,n3)\, c_{n1,\,n2,\,n}\right]$$

$$= \frac{1}{\left(\sqrt{N}\right)^3} \sum_{k1,k2,k3} [J(k1) + J(k2) + J(k3)]\, e^{i\,(k1\,n1 + k2\,n2 + k3\,n3)}\, c(k1,\,k2,\,k3)$$

If we add the above term to the first term of LHS, we obtain

$$(3\,\epsilon_0 - \epsilon)\, c_{n1,n2,n3} +$$

$$\sum_n \left[J(n-n1)\, c_{n,\,n2,\,n3} + J(n-n2)\, c_{n1,\,n,\,n3} + J(n,\,n3)\, c_{n1,\,n2,\,n}\right]$$

$$= \frac{1}{\left(\sqrt{N}\right)^3} \sum_{k1,k2,k3} \{[\epsilon_0 + J(k1)] + [\epsilon_0 + J(k2)] + [\epsilon_0 + J(k3)] - \epsilon_{trimer}\}$$
$$e^{i\,(k1\,n1 + k2\,n2 + k3\,n3)}\, c(k1,\,k2,\,k3)$$

$$= \frac{1}{\left(\sqrt{N}\right)^3} \sum_{k1,k2,k3} [\epsilon_{exciton}(k1) + \epsilon_{exciton}(k1) + \epsilon_{exciton}(k1) - \epsilon_{trimer}]$$
$$e^{i\,(k1\,n1 + k2\,n2 + k3\,n3)}\, c(k1,\,k2,\,k3)$$

The energy ϵ_{trimer} is for bound or free three – body states

Now consider the term associated with D in LHS

$c_{n1,n2,n3}\,D\,(n1-n2)$

$$= \frac{1}{\left(\sqrt{N}\right)^3}\sum_{k1,k2,k3} c\,(k1,\,k2,\,k3)\,e^{i\,(k1\,n1+k2\,n2+k3\,n3)}\,D\,(n1-n2)$$

$$= \frac{1}{\left(\sqrt{N}\right)^3}\sum_{k1,k2,k3} c\,(k1,\,k2,\,k3)\,e^{i\,(k1\,n1+k2\,n2+k3\,n3)}\,\frac{1}{N}\sum_{q} e^{iq\,(n1-n2)}\,D\,(q)$$

$$= \frac{1}{N\left(\sqrt{N}\right)^3}\sum_{q}\sum_{k1,k2,k3} c\,(k1,\,k2,\,k3)\,e^{i\,(k1+q)\,n1+i\,(k2-q)\,n2+ik3\,n3}\,D\,(q)$$

do some tricks with the index k1, k2 and k3

assume $k1' = k1+q$, $k2' = k2-q$, then

$$= \frac{1}{N\left(\sqrt{N}\right)^3}\sum_{q}\sum_{k1',k2',k3}$$

$$c\,(k1'-q,\,k2'+q,\,k3)\,e^{ik1'\,n1+ik2'\,n2+ik3\,n3}\,D\,(q)$$

$$= \frac{1}{N\left(\sqrt{N}\right)^3}\sum_{q}\sum_{k1,k2,k3}$$

$$c\,(k1-q,\,k2+q,\,k3)\,e^{i\,(k1\,n1+k2\,n2+k3\,n3)}\,D\,(q)$$

Then

$c_{n1,n2,n3}\,[\,D\,(n1-n2)\,+\,D\,(n1-n3)\,+\,D\,(n2-n3)\,]$

$$= \frac{1}{N\left(\sqrt{N}\right)^3}\sum_q \sum_{k1,k2,k3}$$

$$[c(k1-q,\,k2+q,\,k3)+c(k1-q,\,k2,\,k3+q)+c(k1,\,k2-q,\,k3+q)]$$
$$e^{i(k1\,n1+k2\,n2+k3\,n3)}\,D(q)$$

Now the LHS

$$= \frac{1}{\left(\sqrt{N}\right)^3}$$

$$\sum_{k1,k2,k3} e^{i(k1\,n1+k2\,n2+k3\,n3)}\Big\{[\epsilon_{exciton}(k1)+\epsilon_{exciton}(k1)+\epsilon_{exciton}(k1)-\epsilon_{trimer}]$$
$$c(k1,\,k2,\,k3)+\frac{1}{N}\sum_q [c(k1-q,\,k2+q,\,k3)+$$
$$c(k1-q,\,k2,\,k3+q)+c(k1,\,k2-q,\,k3+q)]\,D(q)\Big\}$$

We turn to RHS of the equation

$$2\,\delta_{n1,n2}\sum_n J(n1-n)\,c_{n,\,n2,\,n3}$$

$$= \frac{2}{N}\sum_q e^{iq(n1-n2)}\sum_n J(n1-n)\,\frac{1}{\left(\sqrt{N}\right)^3}\sum_{k1,k2,k3} e^{i(k1\,n+k2\,n2+k3\,n3)}\,c(k1,\,k2,\,k3)$$

$$= \frac{2}{N\left(\sqrt{N}\right)^3}$$

$$\sum_q e^{iq(n1-n2)}\sum_{k1,k2,k3}\sum_n J(n1-n)\,e^{ik1(n-n1)}\,e^{i(k1\,n1+k2\,n2+k3\,n3)}\,c(k1,\,k2,\,k3)$$

$$= \frac{2}{N\left(\sqrt{N}\right)^3}\sum_q e^{iq(n1-n2)}\sum_{k1,k2,k3} J(k1)\,e^{i(k1\,n1+k2\,n2+k3\,n3)}\,c(k1,\,k2,\,k3)$$

$$= \frac{2}{N\left(\sqrt{N}\right)^3}\sum_{k1,k2,k3}\sum_q J(k1)\,e^{i(k1+q)\,n1+i(k2-q)\,n2+i\,k3\,n3}\,c(k1,\,k2,\,k3)$$

Do the same trick as we did for the term associated with D

$$= \frac{2}{N\left(\sqrt{N}\right)^3} \sum_{k1,k2,k3} \sum_{q} J(k1-q)\, e^{i(k1\,n1+k2\,n2+k3\,n3)}\, c(k1-q, k2+q, k3)$$

Therefore, the RHS

$$= \frac{2}{N\left(\sqrt{N}\right)^3} \sum_{k1,k2,k3} \sum_{q} e^{i(k1\,n1+k2\,n2+k3\,n3)} [J(k1-q)\, c(k1-q, k2+q, k3) +$$
$$J(k2-q)\, c(k1, k2-q, k3+q) + J(k3-q)\, c(k1+q, k2+q, k3-q)]$$

Comparing LHS and RHS,

we can obtain the Schrodinger − like equation in k representation

$$[\epsilon_{exciton}(k1) + \epsilon_{exciton}(k1) + \epsilon_{exciton}(k1) - \epsilon_{trimer}]\, c(k1, k2, k3) +$$
$$\frac{1}{N} \sum_{q} [c(k1-q, k2+q, k3) + c(k1-q, k2, k3+q) + c(k1, k2-q, k3+q)]\, D(q)$$

$$= \frac{2}{N} \sum_{q} [J(k1-q)\, c(k1-q, k2+q, k3) +$$
$$J(k2-q)\, c(k1, k2-q, k3+q) + J(k3-q)\, c(k1+q, k2+q, k3-q)]$$