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APPLICATION OF UNITARY TRANSFORMATIONS TO FOURTH ORDER PERTURBATION THEORY

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DEFINITION OF SYMBOLS

Symbol	Definition
$\psi_n^{(0)}$	Unperturbed wave function for the system in the n state
$H^{(0)}$	Unperturbed Hamiltonian
$E_n^{(0)}$	Unperturbed energy eigenvalue
Ψ_n	Wave function for the perturbed system
H	Hamiltonian for the perturbed system
λ	Expansion parameter, such that $\lambda < 1$
$\psi_n^{(i)}$	For $i \neq 0$, these are the wave function corrections for the perturbed system
$H_n^{(i)}$	For $i \neq 0$, these are the perturbation terms in the Hamiltonian
E_n	Energy for the perturbed system
$E_n^{(i)}$	For $i \neq 0$, these are the energy corrections for the perturbed system
$H_{n'n}^{(i)}$	For $i \neq 0$, these are the matrix elements obtained using the unperturbed wave functions
$S_{n'n}^{(i)}$	For $i \neq 0$, these are the matrix elements defining the unitary matrix

APPLICATION OF UNITARY TRANSFORMATIONS TO FOURTH ORDER PERTURBATION THEORY

SUMMARY

Perturbation theory is used to obtain energy corrections to the energy of a nondegenerate stationary system. The unitary transformation method is used to obtain the energy corrections to fourth order. In the first section, a short introduction is given to the usual perturbation techniques. In subsequent sections, the higher order corrections are given in a somewhat detailed manner. The purpose of this approach is to point out the difficulties encountered in using a formalism to obtain useful formulae suitable for numerical calculations.

I. INTRODUCTION

Quantum mechanical problems which can be solved exactly take on the simple form

$$H^{(0)} \psi_n^{(0)} = E_n^{(0)} \psi_n^{(0)} . \tag{1}$$

In this discussion the nondegenerate, stationary type of problem is assumed. The above equation then applies to the unperturbed system, where $H^{(0)}$ is the Hamiltonian. If small perturbations are introduced into the system, the Hamiltonian is usually made up of terms in addition to $H^{(0)}$. In this case equation (1) can no longer be written in closed form, and Ψ is usually found by means of a series expansion made up of successive approximations which are denoted by $\psi^{(n)}$, thus

$$\Psi_n = \psi_n^{(0)} + \lambda \psi_n^{(1)} + \lambda^2 \psi_n^{(2)} + \ldots, \quad \lambda < 1 . \tag{2}$$

Here λ is a small parameter which goes to zero when the perturbation is removed. The above wave function then corresponds to a modified Hamiltonian

$$H = H^{(0)} + \lambda H^{(1)} + \lambda^2 H^{(2)} + \ldots \quad . \tag{3}$$

In the above expression, the Hamiltonian terms due to the perturbation are separated into various factors depending on their magnitude, the larger terms appearing first. In the above formalism, $\psi_n^{(0)}$ is the exact solution to the wave equation when only $H^{(0)}$ appears in the Hamiltonian. If H is separated as indicated, the energy eigenvalue may also be expressed as a series expansion as follows:

$$E_n = E_n^{(0)} + \lambda E_n^{(1)} + \lambda^2 E_n^{(2)} + \ldots \qquad . \tag{4}$$

If one substitutes the above values in Schroedinger's equation, one obtains,

$$(H^{(0)} + \lambda H^{(1)} + \ldots)(\psi_n^{(0)} + \lambda \psi_n^{(1)} + \ldots) = (E_n^{(0)} + \lambda E_n^{(1)} + \ldots)$$

$$\times (\psi_n^{(0)} + \lambda \psi_n^{(1)} + \ldots).$$

At this point one needs to decide how far to carry on the approximation.

A first order approximation includes terms involving λ to the first power, all other terms are neglected. Thus to first order,

$$(H^{(0)} + \lambda H^{(1)})(\psi_n^{(0)} + \lambda \psi_n^{(1)}) = (E_n^{(0)} + \lambda E_n^{(1)})(\psi_n^{(0)} + \lambda \psi_n^{(1)})$$

or

$$(H^{(0)} \psi_n^{(0)} - E_n^{(0)} \psi_n^{(0)}) + \lambda (H^{(1)} \psi_n^{(0)} + H^{(0)} \psi_n^{(1)} - E_n^{(1)} \psi_n^{(0)}$$

$$- E_n^{(0)} \psi_n^{(1)}) = 0.$$

Using equation (1), the first term vanishes. In order for the rest to be true, the λ coefficient must vanish. From the last term above, one gets

$$(H^{(0)} - E_n^{(0)}) \psi_n^{(1)} + (H^{(1)} - E_n^{(1)}) \psi_n^{(0)} = 0.$$

Operating on the above equation as follows, one obtains

$$(\psi_m^{(0)} \mid H^{(0)} - E_n^{(0)} \mid \psi_n^{(1)}) + (\psi_m^{(0)} \mid H^{(1)} - E_n^{(1)} \mid \psi_n^{(0)}) = 0 \quad ,$$

$$(E_m^{(0)} - E_n^{(0)})\,\delta_{mn} + (\psi_m^{(0)}\,|H^{(1)}|\,\psi_n^{(0)}) = E_n^{(1)}\,\delta_{mn}$$

Since one deals with orthonormal functions, the above simplifies to

$$E_n^{(1)} = (\psi_n^{(0)}\,|H^{(1)}|\,\psi_n^{(0)}) \equiv H_{nn}^{(1)}\ . \tag{5}$$

In integral form one gets the usual form

$$E_n^{(1)} = \int \psi_n^{(0)*}\, H^{(1)}\, \psi_n^{(0)}\, d\tau .$$

In this manner one may obtain all the terms in equation (4) which correspond to the corrections to the energy E_n of the system. For higher order corrections, the algebra rapidly becomes too complex.

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II. APPLICATION OF UNITARY TRANSFORMATIONS

For higher approximations an alternate method [1] is much easier to develop. One simply connects $\psi_n^{(0)}$ with Ψ_n through a unitary transformation and uses a representation in which $H^{(0)}$ forms a diagonal matrix such that

$$(\psi_{n'}^{(0)}\,|H^{(0)}|\,\psi_n^{(0)}) = H_{n'n}^{(0)} = E_n^{(0)}\,\delta_{n'n}\ .$$

With the above requirements, a unitary matrix may be defined such that its elements are given by

$$U_{n'n} = (\psi_{n'}^{(0)}\,|\,1\,|\Psi_n)\ . \tag{6}$$

Using such a matrix, the Hamiltonian of the system in question may be diagonalized by taking

$$H' = U\,H\,U^{-1}\,. \tag{7}$$

After H is diagonalized, the matrix elements of H' are just the required energy corrections.

In order to see how the matrix U is developed, one must recall that the $\psi_n^{(0)}$'s are the basis states corresponding to the unperturbed system, and that the new Ψ's form a new basis corresponding to H. Thus, if one lets

$$\Psi_n = \sum_{j=1}^{N} U^*_{nj}\,\psi_j^{(0)}\,, \tag{8}$$

then one can also write

$$(\Psi_{n'}|\Psi_n) = \delta_{n'n}\,. \tag{9}$$

Substituting equation (8) in equation (9), one obtains

$$\sum_{j=1}^{N}\sum_{i=1}^{N} U_{n'j}\,U^*_{ni}\,(\psi_j^{(0)}|\psi_i^{(0)}) = \delta_{n'n}\,.$$

Simplifying by using the orthonormality condition of the $\psi_n^{(0)}$'s, one obtains

$$\sum_{j=1}^{N} U_{n'j}\,U^*_{nj} = \delta_{n'n}\,,$$

or by using the δ condition explicitly

$$\sum_{j=1}^{N} U_{nj}\,U^*_{nj} = 1.$$

Writing the above in matrix form, one gets

$$U\,U^{\dagger} = 1,$$

which implies that

$$U^{\dagger} = U^{-1} \quad .$$

This condition says that U has an inverse which is equal to its Hermitian conjugate. This U, in turn is a unitary matrix capable of diagonalizing the Hamiltonian H which amounts to solving the problem.

If this method is used in obtaining the energy corrections, the unitary matrix may be written in exponential form. Thus, one can define U as

$$U \equiv e^{iS}, \quad i^2 \equiv -1. \tag{10}$$

S must be a Hermitian matrix ($S = S^{\dagger}$) in this case. With the above definition for U one can easily see that S may be expanded in a series of the form

$$S = \lambda\, S^{(1)} + \lambda^2 S^{(2)} + \ldots \quad . \tag{11}$$

This expansion is such that when λ goes to zero, U becomes the unit matrix as necessary. Before proceeding it is desirable to expand the newly diagonalized Hamiltonian in a similar form, thus

$$H' = E^{(0)} + \lambda\, E^{(1)} + \lambda^2 E^{(2)} + \ldots \quad . \tag{12}$$

H' is expanded in terms of $E^{(n)}$'s because they now correspond to the desired energy corrections in the final result of equation (4)

To obtain the diagonal elements of H'; one starts by substituting equation (10) in equation (7). In addition, an arbitrary parameter (χ) is introduced which will allow the eventual expansion of H' in a Taylor series. Hence, from equation (7) one obtains

$$H' \equiv H(\chi) = e^{i\chi S}\, H\, e^{-i\chi S} \quad . \tag{13}$$

Expanding $H(\chi)$, one gets

$$H(\chi) = H(0) + \left(\frac{dH(\chi)}{d\chi}\right)_{\chi=0} \chi + \frac{1}{2!}\left(\frac{d^2H(\chi)}{d\chi^2}\right)_{\chi=0} \chi^2 + \ldots \quad . \tag{14}$$

When χ goes to zero, H' is still well defined, that is

$$H' = H(0) = H. \tag{15}$$

In order to find the terms of $H(\chi)$, one uses equation (13) to get the indicated derivatives. Remembering that S is independent of χ, one gets

$$\frac{d\,H(\chi)}{d\chi} = i\,S\,e^{i\chi S}\,H\,e^{-i\chi S} + e^{i\chi S}\,H\,e^{-i\chi S}\,(-iS)$$

$$= i(S\,H(\chi) - H(\chi)\,S) \equiv i[S,\ H(\chi)]\ .$$

In the last line the bracket notation is introduced to make things simplier later on. Using the above notation the second derivative is obtained as follows:

$$\frac{d^2\,H(\chi)}{d\chi^2} = \frac{d}{d\chi}\,(i\,[S,\ H(\chi)]) = i\,[S,\ \frac{d\,H(\chi)}{d\chi}]$$

$$= i^2\,[S,\ [S,\ H(\chi)]].$$

In general [2], the α derivative is given by

$$\frac{d^{\alpha}\ H(\chi)}{d\chi^{\alpha}} = i^{\alpha}\ [S,\ [S,\ \ldots\ _{\alpha},\ [S,\ H(\chi)]\ \ldots\ _{\alpha},]].$$

Equation (14) becomes

$$H(\chi) = H(0) + i\,[S,\ H(0)]\ \chi + \frac{i^2}{2!}\,[S,\ [S,\ H(0)]]\ \chi^2 + \ldots\quad .$$

When one lets $\chi = 1$ (its value is arbitrary) and uses equation (15) the above equation becomes

$$H' = H(1) = H + i\,[S,\ H] + \frac{i^2}{2!}\,[S,\ [S,\ H]] + \ldots\quad .$$

By means of equation (13), one sees that H(1) is just H'. To fourth order, H' is given by

$$H' = H + i\,[S,\ H] + \frac{i^2}{2!}\,[S,\ [S,\ H]] + \frac{i^3}{3!}\,[S,\ [S,\ [S,\ H]]]$$
$$+ \frac{i^4}{4!}\,[S,\ [,S,\ [S,\ [S,\ H]]]]. \qquad (16)$$

In subsequent discussions higher order terms will be omitted. Using equations (3) and (11), one obtains for H' the following expression:

$$H' = (H^{(0)} + \lambda H^{(1)} + \lambda^2 H^{(2)} + \ldots)$$

$$+ i [(\lambda S^{(1)} + \lambda^2 S^{(2)} + \ldots), (H^{(0)} + \lambda H^{(1)} + \lambda^2 H^{(2)} + \ldots)]$$

$$+ \frac{i^2}{2!} [(\lambda S^{(1)} + \lambda^2 S^{(2)} + \ldots), [(\lambda S^{(1)} + \lambda^2 S^{(2)} + \ldots),$$

$$(H^{(0)} + \lambda H^{(1)} + \lambda^2 H^{(2)} + \ldots)]]$$

$$+ \frac{i^3}{3!} [S, [S, [S, H]]] + \frac{i^4}{4!} [S, [S, [S, [S, H]]]]. \qquad (16.1)$$

Expanding the first bracket in H' one gets

$$\{[(\lambda S^{(1)} + \lambda^2 S^{(2)} + \lambda^3 S^{(3)} + \lambda^4 S^{(4)}), H^{(0)}]$$

$$+ [(\lambda S^{(1)} + \lambda^2 S^{(2)} + \lambda^3 S^{(3)} + \lambda^4 S^{(4)}), \lambda H^{(1)}]$$

$$+ [(\lambda S^{(1)} + \lambda^2 S^{(2)} + \lambda^3 S^{(3)} + \lambda^4 S^{(4)}), \lambda^2 H^{(2)}]$$

$$+ [(\lambda S^{(1)} + \lambda^2 S^{(2)} + \lambda^3 S^{(3)} + \lambda^4 S^{(4)}), \lambda^3 H^{(3)}]$$

$$+ [(\lambda S^{(1)} + \lambda^2 S^{(2)} + \lambda^3 S^{(3)} + \lambda^4 S^{(4)}), \lambda^4 H^{(4)}]\}.$$

By neglecting all terms in which λ is raised to a power greater than four, one simplifies the above expression and obtains

$$\{[\lambda S^{(1)}, H^{(0)}] + [\lambda^2 S^{(2)}, H^{(0)}] + [\lambda^3 S^{(3)}, H^{(0)}] + [\lambda^4 S^{(4)}, H^{(0)}]$$

$$+ [\lambda S^{(1)}, \lambda H^{(1)}] + [\lambda^2 S^{(2)}, \lambda H^{(1)}] + [\lambda^3 S^{(3)}, \lambda H^{(1)}]$$

$$+ [\lambda S^{(1)}, \lambda^2 H^{(2)}] + [\lambda^2 S^{(2)}, \lambda^2 H^{(2)}] \qquad (B1)$$

$$+ [\lambda S^{(1)}, \lambda^3 H^{(3)}]\}$$

the above expression is written such that it shows how each term is obtained. The first bracket has been evaluated in detail because it is used to evaluate subsequent terms. This can be seen by reference to equation (16). Thus in the calculation of the next bracket in equation (16), use is made of the results obtained for the first bracket as they appear in expression (B1). Expanding, one gets for the next term of equation (16.1), $[(\lambda S^{(1)} + \lambda^2 S^{(2)} + \ldots), \{[S, H]\}]$, the following:

$$\{[\lambda S^{(1)}, \{[\lambda S^{(1)}, H^{(0)}] + [\lambda^2 S^{(2)}, H^{(0)}] + [\lambda^3 S^{(3)}, H^{(0)}] + [\lambda^4 S^{(4)}, H^{(0)}]\}]$$

$$+ [\lambda^2 S^{(2)}, \{[\lambda S^{(1)}, H^{(0)}] + [\lambda^2 S^{(2)}, H^{(0)}] + [\lambda^3 S^{(3)}, H^{(0)}] + [\lambda^4 S^{(4)}, H^{(0)}]\}]$$

$$+ [\lambda^3 S^{(3)}, \{[\lambda S^{(1)}, H^{(0)}] + [\lambda^2 S^{(2)}, H^{(0)}] + [\lambda^3 S^{(3)}, H^{(0)}] + [\lambda^4 S^{(4)}, H^{(0)}]\}]$$

$$+ [\lambda^4 S^{(4)}, \{[\lambda S^{(1)}, H^{(0)}] + [\lambda^2 S^{(2)}, H^{(0)}] + [\lambda^3 S^{(3)}, H^{(0)}] + [\lambda^4 S^{(4)}, H^{(0)}]\}]$$

$$+ [\lambda S^{(1)}, \{[\lambda S^{(1)}, \lambda H^{(1)}] + [\lambda^2 S^{(2)}, \lambda H^{(1)}] + [\lambda^3 S^{(3)}, \lambda H^{(1)}]\}]$$

$$+ [\lambda^2 S^{(2)}, \{[\lambda S^{(1)}, \lambda H^{(1)}] + [\lambda^2 S^{(2)}, \lambda H^{(1)}] + [\lambda^3 S^{(3)}, \lambda H^{(1)}]\}]$$

$$+ [\lambda^3 S^{(3)}, \{[\lambda S^{(1)}, \lambda H^{(1)}] + [\lambda^2 S^{(2)}, \lambda H^{(1)}] + [\lambda^3 S^{(3)}, \lambda H^{(1)}]\}]$$

$$+ [\lambda^4 S^{(4)}, \{[\lambda S^{(1)}, \lambda H^{(1)}] + [\lambda^2 S^{(2)}, \lambda H^{(1)}] + [\lambda^3 S^{(3)}, \lambda H^{(1)}]\}]$$

$$+ [\lambda S^{(1)}, \{[\lambda S^{(1)}, \lambda^2 H^{(2)}] + [\lambda^2 S^{(2)}, \lambda^2 H^{(2)}]\}]$$

$$+ [\lambda^2 S^{(2)}, \{[\lambda S^{(1)}, \lambda^2 H^{(2)}] + [\lambda^2 S^{(2)}, \lambda^2 H^{(2)}]\}]$$

$$+ [\lambda^3 S^{(3)}, \{[\lambda S^{(1)}, \lambda^2 H^{(2)}] + [\lambda^2 S^{(2)}, \lambda^2 H^{(2)}]\}]$$

$$+ [\lambda^4 S^{(4)}, \{[\lambda S^{(1)}, \lambda^2 H^{(2)}] + [\lambda^2 S^{(2)}, \lambda^2 H^{(2)}]\}]$$

$$+ [\lambda S^{(1)}, [\lambda S^{(1)}, \lambda^3 H^{(3)}]]$$

$$+ [\lambda^2 S^{(2)}, [\lambda S^{(1)}, \lambda^3 H^{(3)}]]$$

$$+ [\lambda^3 S^{(3)}, [\lambda S^{(1)}, \lambda^3 H^{(3)}]]$$

$$+ [\lambda^4 S^{(4)}, [\lambda S^{(1)}, \lambda^3 H^{(3)}]]\} .$$

By neglecting terms having λ^n, $n > 4$; one gets for the second bracket in equation (16.1) the following expression:

$$\{[\lambda S^{(1)}, [\lambda S^{(1)}, H^{(0)}]] + [\lambda S^{(1)}, [\lambda^2 S^{(2)}, H^{(0)}]] \quad + [\lambda S^{(1)}, [\lambda^3 S^{(3)}, H^{(0)}]]$$

$$+ [\lambda^2 S^{(2)}, [\lambda S^{(1)}, H^{(0)}]] + [\lambda^2 S^{(2)}, [\lambda^2 S^{(2)}, H^{(0)}]]$$

$$+ [\lambda^3 S^{(3)}, [\lambda S^{(1)}, H^{(0)}]]$$

$$+ [\lambda S^{(1)}, [\lambda S^{(1)}, \lambda H^{(1)}]] + [\lambda S^{(1)}, [\lambda^2 S^{(2)}, \lambda H^{(1)}]] \tag{B2}$$

$$+ [\lambda^2 S^{(2)}, [\lambda S^{(1)}, \lambda H^{(1)}]]$$

$$+ [\lambda S^{(1)}, [\lambda S^{(1)}, \lambda^2 H^{(2)}]]\} .$$

Clearly the last factors on each one of the lines in expression (B1) did not contribute to expression (B2). Hence, in the calculation of the third bracket in equation (16), the last factors on each one of the lines of expression (B2) will be left out. With this in mind, the third bracket of equation (16) is obtained as follows:

By taking

$$[(\lambda S^{(1)} + \lambda^2 S^{(2)} + \ldots), \{[S, [S,H]]\}],$$

and by substituting the appropriate terms in expression (B2), one obtains

$$\{[\lambda S^{(1)}, \{[\lambda S^{(1)}, [\lambda S^{(1)}, H^{(0)}]] + [\lambda S^{(1)}, [\lambda^2 S^{(2)}, H^{(0)}]]\}]$$

$$+ [\lambda^2 S^{(2)}, \{[\lambda S^{(1)}, [\lambda S^{(1)}, H^{(0)}]] + [\lambda S^{(1)}, [\lambda^2 S^{(2)}, H^{(0)}]]\}]$$

$$+ [\lambda^3 S^{(3)}, \{[\lambda S^{(1)}, [\lambda S^{(1)}, H^{(0)}]] + [\lambda S^{(1)}, [\lambda^2 S^{(2)}, H^{(0)}]]\}]$$

$$+ [\lambda^4 S^{(4)}, \{[\lambda S^{(1)}, [\lambda S^{(1)}, H^{(0)}]] + [\lambda S^{(1)}, [\lambda^2 S^{(2)}, H^{(0)}]]\}]$$

$$+ [\lambda S^{(1)}, [\lambda^2 S^{(2)}, [\lambda S^{(1)}, H^{(0)}]]]$$

$$+ [\lambda^2 S^{(2)}, [\lambda^2 S^{(2)}, [\lambda S^{(1)}, H^{(0)}]]]$$

$$+ [\lambda^3 S^{(3)}, [\lambda^2 S^{(2)}, [\lambda S^{(1)}, H^{(0)}]]]$$

$$+ [\lambda^4 S^{(4)}, [\lambda^2 S^{(2)}, [\lambda S^{(1)}, H^{(0)}]]]$$

$$+ [\lambda S^{(1)}, [\lambda S^{(1)}, [\lambda S^{(1)}, \lambda H^{(1)}]]]$$

$$+ [\lambda^2 S^{(2)}, [\lambda S^{(1)}, [\lambda S^{(1)}, \lambda H^{(1)}]]]$$

$$+ [\lambda^3 S^{(3)}, [\lambda S^{(1)}, [\lambda S^{(1)}, \lambda H^{(1)}]]]$$

$$+ [\lambda^4 S^{(4)}, [\lambda S^{(1)}, [\lambda S^{(1)}, \lambda H^{(1)}]]]\} .$$

Several terms could have been omitted from the above expression but were retained only for symmetry. Excluding the terms having λ^n for $n > 4$, one derives for the third bracket of equation (16) the following expression:

$$\{[\lambda S^{(1)}, [\lambda S^{(1)}, [\lambda S^{(1)}, H^{(0)}]]] + [\lambda S^{(1)}, [\lambda S^{(1)}, [\lambda^2 S^{(2)}, H^{(0)}]]]$$

$$+ [\lambda^2 S^{(2)}, [\lambda S^{(1)}, [\lambda S^{(1)}, H^{(0)}]]]$$

$$+ [\lambda S^{(1)}, [\lambda^2 S^{(2)}, [\lambda S^{(1)}, H^{(0)}]]]$$

$$+ [\lambda S^{(1)}, [\lambda S^{(1)}, [\lambda S^{(1)}, \lambda H^{(1)}]]]\} . \tag{B3}$$

For reasons previously stated, only the first term in expression (B3) contributes to the fourth bracket. From equation (16) and expression (B3) there results the following expression for the last bracket in equation (16):

$$[(\lambda S^{(1)} + \lambda^2 S^{(2)} + \ldots), [\lambda S^{(1)}, [\lambda S^{(1)}, [\lambda S^{(1)}, H^{(0)}]]]].$$

If this term is expanded, only the first factor is retained, i.e.,

$$[\lambda S^{(1)}, [\lambda S^{(1)}, [\lambda S^{(1)}, [\lambda S^{(1)}, H^{(0)}]]]]. \tag{B4}$$

Incorporating the expressions found (B1, B2, B3, B4) for the various brackets in equation (16.1) H' becomes

$$
\begin{aligned}
H' = {} & H^{(0)} + \lambda H^{(1)} + \lambda^2 H^{(2)} + \lambda^3 H^{(3)} + \lambda^4 H^{(4)} \\
& + i\{\lambda [S^{(1)}, H^{(0)}] + \lambda^2 ([S^{(2)}, H^{(0)}] + [S^{(1)}, H^{(1)}]) \\
& \quad + \lambda^3 ([S^{(3)}, H^{(0)}] + [S^{(2)}, H^{(1)}] + [S^{(1)}, H^{(2)}]) \\
& \quad + \lambda^4 ([S^{(4)}, H^{(0)}] + [S^{(3)}, H^{(1)}] + [S^{(2)}, H^{(2)}] + [S^{(1)}, H^{(3)}])\} \\
& + \frac{i^2}{2!}\{\lambda^2 [S^{(1)}, [S^{(1)}, H^{(0)}]] + \lambda^3 ([S^{(1)}, [S^{(2)}, H^{(0)}]] \\
& \quad + [S^{(2)}, [S^{(1)}, H^{(0)}]] + [S^{(1)}, [S^{(1)}, H^{(1)}]]) \\
& \quad + \lambda^4 ([S^{(1)}, [S^{(3)}, H^{(0)}]] + [S^{(2)}, [S^{(2)}, H^{(0)}]] + [S^{(3)}, [S^{(1)}, H^{(0)}]] \\
& \quad + [S^{(1)}, [S^{(2)}, H^{(1)}]] + [S^{(2)}, [S^{(1)}, H^{(1)}]] + [S^{(1)}, [S^{(1)}, H^{(2)}]])\} \\
& + \frac{i^3}{3!}\{\lambda^3 [S^{(1)}, [S^{(1)}, [S^{(1)}, H^{(0)}]]] + \lambda^4 ([S^{(1)}, [S^{(1)}, [S^{(2)}, H^{(0)}]]] \\
& \quad + [S^{(2)}, [S^{(1)}, [S^{(1)}, H^{(0)}]]] + [S^{(1)}, [S^{(2)}, [S^{(1)}, H^{(0)}]]] \\
& \quad + [S^{(1)}, [S^{(1)}, [S^{(1)}, H^{(1)}]]])\} \\
& \quad + \frac{i^4}{4!}\{\lambda^4 [S^{(1)}, [S^{(1)}, [S^{(1)}, [S^{(1)}, H^{(0)}]]]]\}.
\end{aligned}
$$

To solve for the $E_n^{(i)}$ elements one compares the equation above with equation (12) and simply equates coefficients of the various powers in λ. Hence, one obtains the following equations:

$$E^{(0)} = H^{(0)}, \tag{17}$$

$$E^{(1)} = H^{(1)} + i\,[S^{(1)}, H^{(0)}], \tag{18}$$

$$E^{(2)} = H^{(2)} + i\,([S^{(2)}, H^{(0)}] + [S^{(1)}, H^{(1)}]) + \frac{i^2}{2!}[S^{(1)}, [S^{(1)}, H^{(0)}]], \tag{19}$$

$$\begin{aligned} E^{(3)} = {} & H^{(3)} + i\,([S^{(3)}, H^{(0)}] + [S^{(2)}, H^{(1)}] + [S^{(1)}, H^{(2)}]) \\ & + \frac{i^2}{2!}([S^{(1)}, [S^{(2)}, H^{(0)}]] + [S^{(2)}, [S^{(1)}, H^{(0)}]] + [S^{(1)},[S^{(1)},H^{(1)}]]) \\ & + \frac{i^3}{3!}[S^{(1)}, [S^{(1)}, [S^{(1)}, H^{(0)}]]], \end{aligned} \tag{20}$$

$$\begin{aligned} E^{(4)} = {} & H^{(4)} + i\,([S^{(4)}, H^{(0)}] + [S^{(3)}, H^{(1)}] + [S^{(2)}, H^{(2)}] + [S^{(1)}, H^{(3)}]) \\ & + \frac{i^2}{2!}([S^{(1)}, [S^{(3)}, H^{(0)}]] + [S^{(2)}, [S^{(2)}, H^{(0)}]] + [S^{(3)}, [S^{(1)}, H^{(0)}]] \\ & \qquad + [S^{(1)}, [S^{(2)}, H^{(1)}]] + [S^{(2)}, [S^{(1)}, H^{(1)}]] + [S^{(1)},[S^{(1)},H^{(2)}]]) \\ & + \frac{i^3}{3!}([S^{(1)}, [S^{(1)}, [S^{(2)}, H^{(0)}]]] + [S^{(1)}, [S^{(2)}, [S^{(1)}, H^{(0)}]]] \\ & \qquad + [S^{(1)}, [S^{(1)}, [S^{(1)}, H^{(1)}]]] + [S^{(2)}, [S^{(1)},[S^{(1)}, H^{(0)}]]]) \\ & + \frac{i^4}{4!}[S^{(1)}, [S^{(1)}, [S^{(1)}, [S^{(1)}, H^{(0)}]]]] \, . \end{aligned} \tag{21}$$

III. FIRST AND SECOND ORDER FORMULAS

In the preceding section, formulas were derived for the first four corrections to the energy of a perturbed system. These equations will now be expressed in terms of specific matrix elements. This is the final step in obtaining actual energy corrections in analytical form, because the wave functions which are solutions to the unperturbed problem are used in evaluating these matrix elements.

Since one uses a matrix representation in which $H^{(0)}$ is a diagonal matrix, equation (17) is simply an identity, that is,

$$E_n^{(0)} \delta_{n'n} = H_{n'n}^{(0)} .$$

Writing equation (18) in matrix form, one obtains*

$$E_n^{(1)} \delta_{n'n} = H_{n'n}^{(1)} + i \sum_{n''} (S_{n'n''}^{(1)} H_{n''n}^{(0)} - H_{n'n''}^{(0)} S_{n''n}^{(1)})$$

$$= H_{n'n}^{(1)} + i \, (E_n^{(0)} - E_{n'}^{(0)}) \, S_{n'n}^{(1)} \quad . \qquad (22)$$

Since only the diagonal terms are desired, one can simplify the above expression to

$$E_n^{(1)} = H_{nn}^{(1)} .$$

As expected, this result agrees with equation (5).

Starting from equation (19), one obtains the second order formula as follows: Take equation (18) and solve for $[S^{(1)}, H^{(0)}]$. Substitute this value in equation (19). With this modification, $E^{(2)}$ becomes

$$E_n^{(2)} \delta_{n'n} = H_{n'n}^{(2)} + i \left([S^{(2)}, H^{(0)}] + \frac{1}{2} [S^{(1)}, H^{(1)}] + \frac{1}{2} [S^{(1)}, E^{(1)}] \right)_{n'n} . \qquad (23)$$

The diagonal terms are obtained as follows: Let $n' = n$, then

---

* Use is made of the matrix multiplication rules;

$$c_{kj} = \sum_i b_{ki} \, a_{ij} \quad \text{and} \quad d_{lm} = \sum_i \sum_j a_{li} \, b_{ij} \, c_{jm}$$

$$E_n^{(2)} = H_{nn}^{(2)} + i \sum_{n'} \{ (S_{nn'}^{(2)} H_{n'n}^{(0)} - H_{nn'}^{(0)} S_{n'n}^{(2)})$$

$$+ \frac{1}{2} (S_{nn'}^{(1)} H_{n'n}^{(1)} - H_{nn'}^{(1)} S_{n'n}^{(1)}) + \frac{1}{2} (S_{nn'}^{(1)} E_n^{(1)} \delta_{n'n} - E_{n'}^{(1)} \delta_{nn'} S_{n'n}^{(1)}) \}.$$

By replacing $H^{(0)}$ by $E_n^{(0)} \delta_{n'n}$ and by recalling that $E_n^{(1)}$ is a diagonal matrix, one can reduce the above equation to this form:

$$E_n^{(2)} = H_{nn}^{(2)} + \frac{i}{2} \sum_{n'} (S_{nn'}^{(1)} H_{n'n}^{(1)} - H_{nn'}^{(1)} S_{n'n}^{(1)}) . \tag{24}$$

To solve for $E_n^{(2)}$ in terms of known matrix elements, one needs to obtain an expression for $S_{n'n}^{(1)}$. This can be accomplished by using the nondiagonal terms of equation (22). For $n' \neq n$, one obtains*

$$0 = H_{n'n}^{(1)} + i (E_n^{(0)} - E_{n'}^{(0)}) S_{n'n}^{(1)} ,$$

or

$$S_{n'n}^{(1)} = \frac{i H_{n'n}^{(1)}}{(E_n^0 - E_{n'}^0)} , \qquad n' \neq n. \tag{25}$$

Since only the nondegenerate case is being treated no problems are encountered with denominators of the type encountered in equation (25) and subsequent work. When $S_{n'n}^{(1)}$ is substituted in equation (24), one gets

$$E_n^{(2)} = H_{nn}^{(2)} + \frac{i}{2} \sum_{n' \neq n} \left(\frac{H_{nn'}^{(1)} H_{n'n}^{(1)}}{i (E_n^0 - E_{n'}^0)} - \frac{H_{nn'}^{(1)} H_{n'n}^{(1)}}{i (E_{n'}^0 - E_n^0)} \right) ,$$

and by rearranging terms,

$$E_n^{(2)} = H_{nn}^{(2)} + \sum_{n' \neq n} \frac{H_{nn'}^{(1)} H_{n'n}^{(1)}}{(E_n^0 - E_{n'}^0)} . \tag{26}$$

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* In the discussion that follows, the parenthesis around the zero in $E_n^{(0)}$ will be dropped to simplify the notation.

This result can easily be verified by extension of the method outlined in the introduction. To solve for $E_n^{(k)}$, one is required to know $S_{n'n}^{(k-1)}$. This will always be the case. In the next section, for instance, to solve for $E_n^{(3)}$ one needs to know $S_{n'n}^{(2)}$.

IV. THIRD ORDER FORMULAS

So far, the formulas derived are not too difficult, and any method is equally suitable. For the third order corrections, the present method appears to have certain advantages. To solve for $E_n^{(3)}$, one substitutes values for $[S^{(2)}, H^{(0)}]$ and $[S^{(1)}, H^{(0)}]$ in terms of $E_n^{(2)}$ and $E_n^{(1)}$. From equations (18) and (19), one obtains

$$[S^{(1)}, H^{(0)}] = \frac{(E^{(1)} - H^{(1)})}{i} \quad ,$$

$$[S^{(2)}, H^{(0)}] = \frac{(E^{(2)} - H^{(2)})}{i} - \frac{1}{2}[S^{(1)}, H^{(1)}] - \frac{1}{2}[S^{(1)}, E^{(1)}].$$

After substituting these values into equation (20) and rearranging factors, equation (20) becomes

$$E^{(3)} = H^{(3)} + i\,([S^{(3)}, H^{(0)}] + \frac{1}{2}[S^{(2)}, H^{(1)}] + \frac{1}{2}[S^{(1)}, H^{(2)}]$$
$$+ \frac{1}{2}[S^{(1)}, E^{(2)}] + \frac{1}{2}[S^{(2)}, E^{(1)}])$$
$$+ \frac{1}{12}([S^{(1)}, [S^{(1)}, E^{(1)}]] - [S^{(1)}, [S^{(1)}, H^{(1)}]]). \tag{27}$$

In order to solve for $E^{(3)}$ in terms of known quantities, it is necessary to obtain $S_{n'n}^{(2)}$. Taking the nondiagonal terms of equation (23) one obtains

$$0 = H^{(2)}_{n'n} + i\left([S^{(2)}, H^{(0)}] + \frac{1}{2}[S^{(1)}, H^{(1)}] + \frac{1}{2}[S^{(1)}, E^{(1)}]\right)_{n'n} .$$

Using

$$H^{(1)}_{n'n} = E^{(1)}_{n}\,\delta_{n'n} \quad , \qquad\qquad H^{(0)}_{nn} = E^{0}_{n} \quad ,$$

one obtains

$$0 = H^{(2)}_{n'n} + i\,(E^{0}_{n} - E^{0}_{n'})\,S^{(2)}_{n'n} + \frac{i}{2}\,(E^{(1)}_{n} - E^{(1)}_{n'})\,S^{(1)}_{n'n}$$

$$+ \frac{i}{2}\sum_{n''}\left(S^{(1)}_{n'n''}H^{(1)}_{n''n} - H^{(1)}_{n'n''}S^{(1)}_{n''n}\right).$$

After substituting for $S^{(1)}_{n'n}$ and solving for $S^{(2)}_{n'n}$ one obtains (for $n' \neq n$)

$$S^{(2)}_{n'n} = \frac{i\,H^{(2)}_{n'n}}{(E^{0}_{n} - E^{0}_{n'})} + \frac{i}{2}\,\frac{H^{(1)}_{n'n}\,(H^{(1)}_{n'n'} - H^{(1)}_{nn})}{(E^{0}_{n} - E^{0}_{n'})^{2}}$$

$$\frac{i}{2}\sum_{n''\neq n,\,n'}^{*}\frac{H^{(1)}_{n'n''}\,H^{(1)}_{n''n}}{(E^{0}_{n} - E^{0}_{n'})}\left(\frac{1}{E^{0}_{n} - E^{0}_{n''}} + \frac{1}{E^{0}_{n'} - E^{0}_{n''}}\right) \quad . \tag{28}$$

The above solution for $S^{(2)}_{n'n}$ determines only the nondiagonal terms. The diagonal terms are arbitrary and are not important in the energy corrections. These terms affect only the phase relations of the wave function corrections $\psi_n^{(i)}$. The $(*)$ in the last term in $S^{(2)}_{n'n}$ indicates that, when this term is multiplied out, the factor corresponding to $n'' = n$ is left out in the first term and the factor corresponding to $n'' = n'$ is left out in the second term. Having obtained $S^{(2)}_{n'n}$, one proceeds to calculate $E^{(3)}_{n}$. One obtains the diagonal terms from equation (27). By using the diagonal properties of $E^{(i)}$, only the following terms remain

$$E_n^{(3)} = H_{nn}^{(3)} + \frac{i}{2} \sum_{n'} \{(S_{nn'}^{(2)} H_{n'n}^{(1)} - H_{nn'}^{(1)} S_{n'n}^{(2)}) + (S_{nn'}^{(1)} H_{n'n}^{(2)} - H_{nn'}^{(2)} S_{n'n}^{(1)})\}$$

$$- \frac{1}{12} ([S^{(1)}, [S^{(1)}, H^{(1)}]] - [S^{(1)}, [S^{(1)}, E^{(1)}]])_{nn} . \qquad (29)$$

In order to calculate the above, one must substitute for $S_{n'n}^{(2)}$ and $S_{n'n}^{(1)}$. Each term in equation (29) is obtained separately, as follows:

The second term is

$$\sum_{n' \neq n} \left\{ \frac{i^2}{2} \left(\frac{H_{nn'}^{(2)} H_{n'n}^{(1)}}{(E_{n'}^0 - E_n^0)} - \frac{H_{nn'}^{(1)} H_{n'n}^{(2)}}{(E_n^0 - E_{n'}^0)} \right) \right.$$

$$\left. + \frac{i^2}{4} \left(\frac{H_{nn'}^{(1)} (H_{nn}^{(1)} - H_{n'n'}^{(1)}) H_{n'n}^{(1)}}{(E_{n'}^0 - E_n^0)^2} - \frac{H_{nn'}^{(1)} H_{n'n}^{(1)} (H_{n'n'}^{(1)} - H_{nn}^{(1)})}{(E_n^0 - E_{n'}^0)^2} \right) \right\}$$

$$+ \sum_{n' \neq n} \sum_{n'' \neq n, n'}^{*} \frac{i^2}{4} \left\{ \frac{H_{nn''}^{(1)} H_{n''n'}^{(1)} H_{n'n}^{(1)}}{(E_{n'}^0 - E_n^0)} \left(\frac{1}{E_n^0 - E_{n''}^0} + \frac{1}{E_{n'}^0 - E_{n''}^0} \right) \right.$$

$$\left. - \frac{H_{nn'}^{(1)} H_{n'n''}^{(1)} H_{n''n}^{(1)}}{(E_n^0 - E_{n'}^0)} \left(\frac{1}{E_{n'}^0 - E_{n''}^0} + \frac{1}{E_n^0 - E_{n''}^0} \right) \right\} .$$

Simplifying this term, one gets

$$\frac{1}{2} \sum_{n' \neq n} \left\{ \frac{(H_{nn'}^{(2)} H_{n'n}^{(1)} + H_{nn'}^{(1)} H_{n'n}^{(2)})}{(E_n^0 - E_{n'}^0)} + \frac{H_{nn'}^{(1)} H_{n'n}^{(1)} (H_{n'n'}^{(1)} - H_{nn}^{(1)})}{(E_n^0 - E_{n'}^0)^2} \right\}$$

$$+\frac{1}{4}\sum_{n'\neq n}\sum_{n''\neq n,n'}^{*}\frac{(H^{(1)}_{nn''}H^{(1)}_{n''n'}H^{(1)}_{n'n}+H^{(1)}_{nn'}H^{(1)}_{n'n''}H^{(1)}_{n''n})}{(E^0_n-E^0_{n'})}$$

$$\times\left(\frac{1}{E^0_n-E^0_{n''}}+\frac{1}{E^0_{n'}-E^0_{n''}}\right). \tag{29.2}$$

The third term is

$$\frac{i}{2}\sum_{n'\neq n}\left(\frac{H^{(1)}_{nn'}H^{(2)}_{n'n}}{i(E^0_n-E^0_{n'})}-\frac{H^{(2)}_{nn'}H^{(1)}_{n'n}}{i(E^0_{n'}-E^0_n)}\right)=\frac{1}{2}\sum_{n'\neq n}\frac{(H^{(2)}_{nn'}H^{(1)}_{n'n}+H^{(1)}_{nn'}H^{(2)}_{n'n})}{(E^0_n-E^0_{n'})}. \tag{29.3}$$

The fourth term is

$$\left(-\frac{1}{12}S^{(1)}S^{(1)}H^{(1)}+\frac{1}{6}S^{(1)}H^{(1)}S^{(1)}-\frac{1}{12}H^{(1)}S^{(1)}S^{(1)}\right)_{nn}.$$

Substituting for $S^{(1)}_{n'n}$, one obtains

$$\frac{1}{12}\sum_{n'\neq n}\sum_{n''\neq n'}\frac{H^{(1)}_{nn'}H^{(1)}_{n'n''}H^{(1)}_{n''n}}{(E^0_n-E^0_{n'})(E^0_{n'}-E^0_{n''})}+\frac{1}{6}\sum_{n'\neq n}\sum_{n''\neq n}\frac{H^{(1)}_{nn'}H^{(1)}_{n'n''}H^{(1)}_{n''n}}{(E^0_n-E^0_{n'})(E^0_n-E^0_{n''})}$$

$$+\frac{1}{12}\sum_{n'\neq n}\sum_{n''\neq n'}\frac{H^{(1)}_{nn''}H^{(1)}_{n''n'}H^{(1)}_{n'n}}{(E^0_n-E^0_{n'})(E^0_{n'}-E^0_{n''})}.$$

The last factor was obtained by interchanging n' and n". Further simplification can be accomplished by breaking up the "1/6" term into two "1/12" terms and interchanging n" and n' in one of these terms before combining with the other two terms. By the above manipulation, the fourth term becomes

$$\frac{1}{12}\sum_{n'\neq n}\ \sum^{*}_{n''\neq n,n'}\frac{(H^{(1)}_{nn'}H^{(1)}_{n'n''}H^{(1)}_{n''n}+H^{(1)}_{nn''}H^{(1)}_{n''n'}H^{(1)}_{n'n})}{(E^0_n-E^0_{n'})}$$

$$\times\left(\frac{1}{E^0_n-E^0_{n''}}+\frac{1}{E^0_{n'}-E^0_{n''}}\right)\ . \qquad (29.4)$$

The last term is

$$\left(\frac{1}{12}S^{(1)}S^{(1)}E^{(1)}-\frac{1}{6}S^{(1)}E^{(1)}S^{(1)}+\frac{1}{12}E^{(1)}S^{(1)}S^{(1)}\right)_{nn}.$$

Substituting for $S^{(1)}_{n'n}$ one gets

$$\sum_{n'\neq n}\left(\frac{1}{12}\frac{H^{(1)}_{nn'}H^{(1)}_{n'n}E^{(1)}_{n}}{(E^0_n-E^0_{n'})^2}-\frac{1}{6}\frac{H^{(1)}_{nn'}H^{(1)}_{n'n}E^{(1)}_{n'}}{(E^0_n-E^0_{n'})^2}+\frac{1}{12}\frac{H^{(1)}_{nn'}H^{(1)}_{n'n}E^{(1)}_{n}}{(E^0_n-E^0_{n'})^2}\right),$$

which, when combined, becomes

$$-\frac{1}{6}\sum_{n'\neq n}\frac{H^{(1)}_{nn'}H^{(1)}_{n'n}(H^{(1)}_{n'n'}-H^{(1)}_{nn})}{(E^0_n-E^0_{n'})^2}\ . \qquad (29.5)$$

When all the above terms are collected, one obtains for $E^{(3)}_n$:

$$E^{(3)}_n=H^{(3)}_{nn}+\sum_{n'\neq n}\left\{\frac{(H^{(2)}_{nn'}H^{(1)}_{n'n}+H^{(1)}_{nn'}H^{(2)}_{n'n})}{(E^0_n-E^0_{n'})}+\frac{1}{3}\frac{H^{(1)}_{nn'}H^{(1)}_{n'n}(H^{(1)}_{n'n'}-H^{(1)}_{nn})}{(E^0_n-E^0_{n'})^2}\right\}$$

$$+\frac{1}{3}\sum_{n'\neq n}\ \sum^{*}_{n''\neq n,n'}\frac{(H^{(1)}_{nn'}H^{(1)}_{n'n''}H^{(1)}_{n''n}+H^{(1)}_{nn''}H^{(1)}_{n''n'}H^{(1)}_{n'n})}{(E^0_n-E^0_{n'})}$$

$$\times\left(\frac{1}{E^0_n-E^0_{n''}}+\frac{1}{E^0_{n'}-E^0_{n''}}\right) \qquad (30)$$

The preceding result may be simplified by modifying the last term so that the double sum will be symmetric in n' as well as n''. This is accomplished as follows: Express the last term as a sum of two terms in the order in which they appear; then from each take out a factor corresponding to n'' = n' and n'' = n respectively. After the indicated factor is removed, the first factor becomes

$$\frac{1}{3} \sum_{n' \neq n} \sum_{n'' \neq n, n'} \frac{(H^{(1)}_{nn'} H^{(1)}_{n'n''} H^{(1)}_{n''n} + H^{(1)}_{nn''} H^{(1)}_{n''n'} H^{(1)}_{n'n})}{(E^0_n - E^0_{n'})(E^0_n - E^0_{n''})}$$

$$+ \frac{2}{3} \sum_{n' \neq n} \frac{(H^{(1)}_{nn'} H^{(1)}_{n'n}) H^{(1)}_{n'n'}}{(E^0_n - E^0_{n'})^2} ,$$

and the second factor becomes

$$\frac{1}{3} \sum_{n' \neq n} \sum_{n'' \neq n, n'} \frac{(H^{(1)}_{nn'} H^{(1)}_{n'n''} H^{(1)}_{n''n} + H^{(1)}_{nn''} H^{(1)}_{n''n'} H^{(1)}_{n'n})}{(E^0_n - E^0_{n'})(E^0_{n'} - E^0_{n''})}$$

$$- \frac{2}{3} \sum_{n' \neq n} \frac{(H^{(1)}_{nn'} H^{(1)}_{n'n}) H^{(1)}_{nn}}{(E^0_n - E^0_{n'})^2} .$$

Note that the last two terms of the above expressions combine with the third term of equation (30). Thus, equation (30) is modified as follows* :

$$E^{(3)}_n = H^{(3)}_{nn} + \sum_{n' \neq n} \left\{ \frac{(H^{(2)}_{nn'} H^{(1)}_{n'n} + H^{(1)}_{nn'} H^{(2)}_{n'n})}{(E^0_n - E^0_{n'})} + \frac{H^{(1)}_{nn'} H^{(1)}_{n'n} (H^{(1)}_{n'n'} - H^{(1)}_{nn})}{(E^0_n - E^0_{n'})^2} \right\}$$

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* This result agrees with equation (11-33) in Powell and Crasemann's book on Quantum Mechanics.

$$+\frac{1}{3}\sum_{n'\neq n}\sum_{n''\neq n,n'}\frac{(H^{(1)}_{nn'}H^{(1)}_{n'n''}H^{(1)}_{n''n}+H^{(1)}_{nn''}H^{(1)}_{n''n'}H^{(1)}_{n'n})}{(E^0_n-E^0_{n'})}$$

$$\times\left(\frac{1}{E^0_n-E^0_{n''}}+\frac{1}{E^0_{n'}-E^0_{n''}}\right) \quad . \qquad (31)$$

A more compact form is obtained by expressing the double summations in a different manner. Take the above term and write it as two terms after interchanging n'' and n' in one of them. This gives

$$\frac{1}{3}\sum_{n'\neq n}\sum_{n''\neq n,n'}\frac{H^{(1)}_{nn'}H^{(1)}_{n'n''}H^{(1)}_{n''n}}{(E^0_n-E^0_{n'})}\left(\frac{1}{E^0_n-E^0_{n''}}+\frac{1}{E^0_{n'}-E^0_{n''}}\right)$$

$$+\frac{1}{3}\sum_{n'\neq n}\sum_{n''\neq n,n'}\frac{H^{(1)}_{nn'}H^{(1)}_{n'n''}H^{(1)}_{n''n}}{(E^0_n-E^0_{n''})}\left(\frac{1}{E^0_n-E^0_{n'}}+\frac{1}{E^0_{n''}-E^0_{n'}}\right) .$$

Combining these two terms again one gets

$$\frac{1}{3}\sum_{n'\neq n}\sum_{n''\neq n,n'}H^{(1)}_{nn'}H^{(1)}_{n'n''}H^{(1)}_{n''n}\left\{\frac{(E^0_n+E^0_{n'}-2E^0_{n''})+(2E^0_{n'}-E^0_n-E^0_{n''})}{(E^0_n-E^0_{n'})(E^0_n-E^0_{n''})(E^0_{n'}-E^0_{n''})}\right\}$$

$$=\sum_{n'\neq n}\sum_{n''\neq n,n'}\frac{H^{(1)}_{nn'}H^{(1)}_{n'n''}H^{(1)}_{n''n}}{(E^0_n-E^0_{n'})(E^0_n-E^0_{n''})} \quad .$$

Now, one puts back the factor corresponding to n'' = n' in the above expression and obtains

$$\sum_{n'\neq n}\sum_{n''\neq n}\frac{H^{(1)}_{nn'}H^{(1)}_{n'n''}H^{(1)}_{n''n}}{(E^0_n-E^0_{n'})(E^0_n-E^0_{n''})}-\sum_{n'\neq n}\frac{(H^{(1)}_{nn'}H^{(1)}_{n'n})H^{(1)}_{n'n'}}{(E^0_n-E^0_{n'})^2} \quad .$$

When this result is substituted in equation (31), the following is obtained:

$$E_n^{(3)} = H_{nn}^{(3)} + \sum_{n'\neq n} \frac{(H_{nn'}^{(1)} H_{n'n}^{(2)} + H_{nn'}^{(2)} H_{n'n}^{(1)})}{(E_n^0 - E_{n'}^0)} - H_{nn}^{(1)} \sum_{n'\neq n} \frac{H_{nn'}^{(1)} H_{n'n}^{(1)}}{(E_n^0 - E_{n'}^0)^2}$$

$$+ \sum_{n'\neq n} \sum_{n''\neq n} \frac{H_{nn'}^{(1)} H_{n'n''}^{(1)} H_{n''n}^{(1)}}{(E_n^0 - E_{n'}^0)(E_n^0 - E_{n''}^0)} \quad . \qquad (32)$$

The above result is easier to use in actual calculations.

V. FOURTH ORDER FORMULAS

In this section, the expression for $E_n^{(4)}$ is derived. From the general form developed in Section II, one obtains the fourth order correction to the energy. As was the case for $E_n^{(3)}$, one needs to substitute known quantities for $[S^{(1)}, H^{(0)}]$, $[S^{(2)}, H^{(0)}]$, and $[S^{(3)}, H^{(0)}]$. Some of these quantities were defined in the preceding section. From equation (27) one solves for the remaining expression:

$$[S^{(3)}; H^{(0)}] = \frac{(E^{(3)} - H^{(3)})}{i} - \frac{1}{2}([S^{(2)}, H^{(1)}] + [S^{(1)}, H^{(2)}] + [S^{(2)}, E^{(1)}]$$

$$+ [S^{(1)}, E^{(2)}]) - \frac{i}{12}([S^{(1)}, [S^{(1)}, H^{(1)}]]$$

$$- [S^{(1)}, [S^{(1)}, E^{(1)}]]). \qquad (33)$$

In equation (21) note that the term above is also found within brackets. Hence, in addition to the above, one needs to calculate $[S^{(1)}, [S^{(3)}, H^{(0)}]]$. The expression for this term is

$$\{[S^{(1)}, \frac{E^{(3)}}{i}] - [S^{(1)}, \frac{H^{(3)}}{i}] - \frac{1}{2}([S^{(1)}, [S^{(2)}, H^{(1)}]] + [S^{(1)}, [S^{(1)}, H^{(2)}]]$$

$$+ [S^{(1)}, [S^{(2)}, E^{(1)}]] + [S^{(1)}, [S^{(1)}, E^{(2)}]])$$

$$- \frac{i}{12} ([S^{(1)},[S^{(1)},[S^{(1)}, H^{(1)}]]] - [S^{(1)},[S^{(1)},[S^{(1)}, E^{(1)}]]])\} \ .$$

With the above expressions substituted into equation (21), $E^{(4)}$ becomes

$$E^{(4)} = H^{(4)} + i\{[S^{(4)},H^{(0)}] + [S^{(3)} H^{(1)}] + [S^{(2)}, H^{(2)}] + [S^{(1)}, H^{(3)}]\}$$

$$+ \frac{i}{2}[S^{(1)},E^{(3)}] - \frac{i}{2}[S^{(1)},H^{(3)}] + \frac{1}{4}[S^{(1)}[S^{(2)},H^{(1)}]] + \frac{1}{4}[S^{(1)},[S^{(1)}, H^{(2)}]]$$

$$+ \frac{1}{4}[S^{(1)},[S^{(2)},E^{(1)}]] + \frac{1}{4}[S^{(1)},[S^{(1)},E^{(2)}]] + \frac{i}{24}[S^{(1)}[S^{(1)}, [S^{(1)}, H^{(1)}]]]$$

$$- \frac{i}{24}[S^{(1)},[S^{(1)},[S^{(1)}, E^{(1)}]]] - \frac{1}{12}[S^{2}, \frac{E^{(2)}}{i}] + \frac{1}{2}[S^{(2)} \frac{H^{(2)}}{i}]$$

$$+ \frac{1}{4}[S^{(2)}, [S^{(1)}, H^{(1)}]] + \frac{1}{4}[S^{(2)}, [S^{(1)}, E^{(1)}]] - \frac{1}{2}[S^{(3)}, \frac{E^{(1)}}{i}] + \frac{1}{2}[S^{(3)},\frac{H^{(1)}}{i}]$$

$$- \frac{1}{12}[S^{(1)},[S^{(2)}, H^{(1)}]] - \frac{1}{2}[S^{(2)},[S^{(1)},H^{(1)}]] - \frac{1}{2}[S^{(1)}, [S^{(1)}, H^{(2)}]]$$

$$- \frac{i}{6}[S^{(1)}[S^{(1)},\frac{E^{(2)}}{i}]] + \frac{i}{6}[S^{(1)},[S^{(1)},\frac{H^{(2)}}{i}]] + \frac{i}{12}[S^{(1)},[S^{(1)},[S^{(1)},H^{(1)}]]]$$

$$+ \frac{i}{12}[S^{(1)}, [S^{(1)}, [S^{(1)}, E^{(1)}]]] - \frac{i}{6}[S^{(1)}, [S^{(2)}, \frac{E^{(1)}}{i}]] + \frac{i}{6}[S^{(1)}, [S^{(2)}, \frac{H^{(1)}}{i}]]$$

$$- \frac{i}{6}[S^{(1)},[S^{(1)},[S^{(1)},H^{(1)}]]] - \frac{i}{6}[S^{(2)},[S^{(1)},\frac{E^{(1)}}{i}]] + \frac{i}{6}[S^{(2)},[S^{(1)},\frac{H^{(1)}}{i}]]$$

$$+ \frac{1}{24}[S^{(1)},[S^{(1)},[S^{(1)},\frac{E^{(1)}}{i}]]] - \frac{1}{24}[S^{(1)},[S^{(1)},[S^{(1)}, \frac{H^{(1)}}{i}]]] \ .$$

Upon recombination, this becomes

$$E^{(4)} = H^{(4)} + \frac{i}{2}\{2[S^{(4)}, H^{(0)}] + [S^{(3)},H^{(1)}] + [S^{(2)}, H^{(2)}] + [S^{(1)}, H^{(3)}]$$

$$+ [S^{(1)}, E^{(3)}] + [S^{(2)}, E^{(2)}] + [S^{(3)}, E^{(1)}]\}$$

$$- \frac{1}{12} \{ [S^{(1)}, [S^{(2)}, H^{(1)}]] + [S^{(1)}, [S^{(1)}, H^{(2)}]]$$

$$- [S^{(1)}, [S^{(2)}, E^{(1)}]] - [S^{(1)}, [S^{(1)}, E^{(2)}]]$$

$$+ [S^{(2)}, [S^{(1)}, H^{(1)}]] - [S^{(2)}, [S^{(1)}, E^{(1)}]] \} . \qquad (34)$$

This result is quite an improvement over the previous expansion.

Once $E_n^{(4)}$ is expressed in its simplest form, the diagonal terms are calculated. Expanding the brackets, one gets the following terms for the diagonal (excluding the zero elements):

$$E_n^{(4)} = H_{nn}^{(4)} + \frac{i}{2} \{ [S^{(3)}, H^{(1)}] + [S^{(2)}, H^{(2)}] + [S^{(1)}, H^{(3)}] \}_{nn}$$

$$+ \frac{1}{12} \{ (S^{(1)} H^{(2)} S^{(1)} + S^{(1)} H^{(2)} S^{(1)}) - (H^{(2)} S^{(1)} S^{(1)} + S^{(1)} S^{(1)} H^{(2)})$$

$$+ (S^{(1)} S^{(1)} E^{(2)} - S^{(1)} E^{(2)} S^{(1)}) + (E^{(2)} S^{(1)} S^{(1)} - S^{(1)} E^{(2)} S^{(1)})$$

$$+ (S^{(2)} H^{(1)} S^{(1)} + S^{(1)} H^{(1)} S^{(2)}) + (S^{(2)} H^{(1)} S^{(1)} + S^{(1)} H^{(1)} S^{(2)})$$

$$- (H^{(1)} S^{(1)} S^{(2)} + S^{(2)} S^{(1)} H^{(1)}) - (S^{(1)} S^{(2)} H^{(1)} + H^{(1)} S^{(2)} S^{(1)})$$

$$+ (S^{(2)} S^{(1)} E^{(1)} + E^{(1)} S^{(1)} S^{(2)}) + (E^{(1)} S^{(2)} S^{(1)} + S^{(1)} S^{(2)} E^{(1)})$$

$$- (S^{(1)} E^{(1)} S^{(2)} + S^{(2)} E^{(1)} S^{(1)}) - (S^{(2)} E^{(1)} S^{(1)} + S^{(1)} E^{(1)} S^{(2)}) \}_{nn} . \qquad (35)$$

Except for $S_{n'n}^{(3)}$, all the terms necessary to calculate $E_n^{(4)}$ have been calculated previously. Before one can continue, $S_{n'n}^{(3)}$ must be obtained. It is obtained from the nondiagonal terms of equation (33). These terms, obtained by expanding equation (33), are:

$$[S^{(3)}, H^{(0)}]_{n'n} = i\,H^{(3)}_{n'n} - \frac{1}{2}\{[S^{(2)}, H^{(1)}] + [S^{(1)}, H^{(2)}] + [S^{(2)}, E^{(1)}]$$

$$+ [S^{(1)}, E^{(2)}]\}_{n'n} + \frac{i}{12}\{(S^{(1)} H^{(1)} S^{(1)} - S^{(1)} S^{(1)} H^{(1)})$$

$$+ (S^{(1)} H^{(1)} S^{(1)} - H^{(1)} S^{(1)} S^{(1)}) + (S^{(1)} S^{(1)} E^{(1)}$$

$$- S^{(1)} E^{(1)} S^{(1)})$$

$$+ (E^{(1)} S^{(1)} S^{(1)} - S^{(1)} E^{(1)} S^{(1)})\}_{n'n} . \tag{36}$$

The above equation is arranged so as to simplify the calculation of $S^{(3)}_{n'n}$. This fact is realized only after trying various combinations. Since

$$[S^{(3)}, H^{(0)}]_{n'n} = \sum_{n''} (S^{(3)}_{n'n''} H^{(0)}_{n''n} - H^{(0)}_{n'n''} S^{(3)}_{n''n})$$

$$= (E^0_n - E^0_{n'}) S^{(3)}_{n'n} ,$$

one can solve for $S^{(3)}_{n'n}$ from equation (36) by simply dividing by $(E^0_n - E^0_{n'})$. This step will be carried out after each term in equation (36) is evaluated.

Before proceeding with the calculation of $S^{(3)}_{n'n}$, one should modify $S^{(2)}_{n'n}$ to simplify matters later on. To do this, one separates the third term of equation (28) into two terms and redefines the resulting terms as follows:

$$\sum_{n''\neq n} \frac{H^{(1)}_{n'n''} H^{(1)}_{n''n}}{(E^0_n - E^0_{n'})(E^0_n - E^0_{n''})} = \left\{ \sum_{n''\neq n, n'} \frac{H^{(1)}_{n'n''} H^{(1)}_{n''n}}{(E^0_n - E^0_{n'})(E^0_n - E^0_{n''})} + \frac{H^{(1)}_{n'n'} H^{(1)}_{n'n}}{(E^0_n - E^0_{n'})^2} \right\}$$

$$\sum_{n''\neq n'} \frac{H^{(1)}_{n'n''} H^{(1)}_{n''n}}{(E^0_n - E^0_{n'})(E^0_{n'} - E^0_{n''})} = \left\{ \sum_{n''\neq n, n'} \frac{H^{(1)}_{n'n''} H^{(1)}_{n''n}}{(E^0_n - E^0_{n'})(E^0_n - E^0_{n''})} - \frac{H^{(1)}_{n'n} H^{(1)}_{nn}}{(E^0_n - E^0_{n'})^2} \right\} .$$

One can see that the factors removed from the sums combine with the second term in equation (28). Incorporating these changes, $S^{(2)}_{n'n}$ becomes

$$S^{(2)}_{n'n} = \frac{i\,H^{(2)}_{n'n}}{(E^0_n - E^0_{n'})} + \frac{i\,H^{(1)}_{n'n}\,(H^{(1)}_{n'n'} - H^{(1)}_{nn})}{(E^0_n - E^0_{n'})^2}$$

$$+ \frac{i}{2} \sum_{n''\neq n, n'} \frac{H^{(1)}_{n'n''}\,H^{(1)}_{n''n}}{(E^0_n - E^0_{n'})} \left(\frac{1}{E^0_n - E^0_{n''}} + \frac{1}{E^0_{n'} - E^0_{n''}} \right) . \quad (37)$$

In Section IV, $E^{(3)}_n$ was obtained without making this modification in $S^{(2)}_{n'n}$. The increased complexity of the present case makes it imperative that this change be made here.

With the modified form of $S^{(2)}_{n'n}$, the calculation of $S^{(3)}_{n'n}$ proceeds smoothly. In the calculation of the terms of equation (36), one will find it more convenient to modify each term as soon as it is calculated. If this is not done, the situation becomes complicated. Taking the second term of equation (36) one obtains the following:

$$-\frac{1}{2}[S^{(2)}, H^{(1)}]_{n'n} \equiv \frac{1}{2} \sum_{n''} (H^{(1)}_{n'n''}\,S^{(2)}_{n''n} - S^{(2)}_{n'n''}\,H^{(1)}_{n''n})$$

$$= \frac{i}{2} \left\{ \sum_{n''\neq n} \frac{H^{(1)}_{n'n''}\,H^{(2)}_{n''n}}{(E^0_n - E^0_{n''})} + \sum_{n''\neq n'} \frac{H^{(2)}_{n'n''}\,H^{(1)}_{n''n}}{(E^0_{n'} - E^0_{n''})} \right.$$

$$\left. + \sum_{n''\neq n} \frac{H^{(1)}_{n'n''}\,H^{(1)}_{n''n}\,(H^{(1)}_{n''n''} - H^{(1)}_{nn})}{(E^0_n - E^0_{n''})^2} + \sum_{n''\neq n'} \frac{H^{(1)}_{n'n''}\,H^{(1)}_{n''n}\,(H^{(1)}_{n''n''} - H^{(1)}_{n'n'})}{(E^0_{n'} - E^0_{n''})^2} \right\}$$

$$+ \frac{i}{4} \left\{ \sum_{n''\neq n} \sum_{n'''\neq n, n''} \frac{H^{(1)}_{n'n''}\,H^{(1)}_{n''n'''}\,H^{(1)}_{n'''n}}{(E^0_n - E^0_{n''})} \left(\frac{1}{(E^0_n - E^0_{n'''})} + \frac{1}{(E^0_{n''} - E^0_{n'''})} \right) \right.$$

$$\left. + \sum_{n''\neq n'} \sum_{n'''\neq n', n''} \frac{H^{(1)}_{n'n'''}\,H^{(1)}_{n'''n''}\,H^{(1)}_{n''n}}{(E^0_{n'} - E^0_{n''})} \left(\frac{1}{E^0_{n'} - E^0_{n'''}} + \frac{1}{E^0_{n''} - E^0_{n'''}} \right) \right\} .$$

By taking out appropriate terms from the above sums, one can write these terms in a more symmetric form. The steps necessary for this modification are as follows: Take out the factors corresponding to $n'' = n'$ in the first term and the one for $n'' = n$ in the second term, this gives

$$\frac{i}{2} \sum_{n''\neq n, n'} \left(\frac{H^{(1)}_{n'n''} H^{(2)}_{n''n}}{(E^0_n - E^0_{n''})} + \frac{H^{(2)}_{n'n''} H^{(1)}_{n''n}}{(E^0_{n'} - E^0_{n''})} \right) + \frac{i}{2} \frac{H^{(2)}_{n'n} (H^{(1)}_{n'n'} - H^{(1)}_{nn})}{(E^0_n - E^0_{n'})} \quad . \tag{a}$$

Repeating this procedure with the next two terms one obtains

$$\frac{i}{2} \sum_{n''\neq n, n'} \left(\frac{H^{(1)}_{n'n''} H^{(1)}_{n''n} (H^{(1)}_{n''n''} - H^{(1)}_{nn})}{(E^0_n - E^0_{n''})^2} + \frac{H^{(1)}_{n'n''} H^{(1)}_{n''n} (H^{(1)}_{n''n''} - H^{(1)}_{n'n'})}{(E^0_{n'} - E^0_{n''})^2} \right)$$

$$+ \frac{i}{2} \frac{H^{(1)}_{n'n} (H^{(1)}_{n'n'} - H^{(1)}_{nn})^2}{(E^0_n - E^0_{n'})^2} \quad . \tag{b}$$

If this step is repeated with the last two terms, the result is

$$\frac{i}{4} \left\{ \sum_{n''\neq n, n'} \sum_{n'''\neq n, n''} \frac{H^{(1)}_{n'n''} H^{(1)}_{n''n'''} H^{(1)}_{n'''n}}{(E^0_n - E^0_{n''})} \left(\frac{1}{E^0_n - E^0_{n'''}} + \frac{1}{E^0_{n''} - E^0_{n'''}} \right) \right.$$

$$\left. + \sum_{n''\neq n, n'} \sum_{n'''\neq n', n''} \frac{H^{(1)}_{n'n'''} H^{(1)}_{n'''n''} H^{(1)}_{n''n}}{(E^0_{n'} - E^0_{n''})} \left(\frac{1}{E^0_{n'} - E^0_{n'''}} + \frac{1}{E^0_{n''} - E^0_{n'''}} \right) \right\}$$

$$+ \frac{i}{4} \sum_{n''\neq n, n'} \frac{H^{(1)}_{n'n''} H^{(1)}_{n''n} (H^{(1)}_{n'n'} - H^{(1)}_{nn})}{(E^0_n - E^0_{n'})} \left(\frac{1}{E^0_n - E^0_{n''}} + \frac{1}{E^0_{n'} - E^0_{n''}} \right) \quad . \tag{c}$$

After the individual terms are obtained by removing terms corresponding to $n'' = n'$ and $n'' = n$ from the main double sums, the last term in (c) is obtained by letting $n''' = n''$. Thus the second term in equation (36) yields terms (a), (b), and (c). These terms will be incorporated with the other terms later on.

The remaining terms of equation (36) are given in their final form only. It is assumed that the reader can retrace the source of the extra terms generated. These terms are:

$$-\frac{1}{2}[S^{(1)}, H^{(2)}]_{n'n} = \frac{i}{2}\sum_{n''\neq n, n'}\left(\frac{H^{(2)}_{n'n''}H^{(1)}_{n''n}}{(E^0_n - E^0_{n''})} + \frac{H^{(1)}_{n'n''}H^{(2)}_{n''n}}{(E^0_{n'} - E^0_{n''})}\right) + \frac{i}{2}\frac{H_{n'n}(H^{(2)}_{n'n'} - H^{(2)}_{nn})}{(E^0_n - E^0_{n'})} \tag{d}$$

$$-\frac{1}{2}[S^{(2)}, E^{(1)}]_{n'n} = \frac{i}{2}\frac{H^{(2)}_{n'n}(E^{(1)}_{n'} - E^{(1)}_{n})}{(E^0_n - E^0_{n'})} + \frac{i}{2}\frac{H^{(1)}_{n'n}(E^{(1)}_{n'} - E^{(1)}_{n})^2}{(E^0_n - E^0_{n'})^2}$$

$$+\frac{i}{4}\sum_{n''\neq n, n'}\frac{H^{(1)}_{n'n''}H^{(1)}_{n''n}(H^{(1)}_{n'n'} - H^{(1)}_{nn})}{(E^0_n - E^0_{n'})}\left(\frac{1}{E^0_n - E^0_{n''}} + \frac{1}{E^0_{n'} - E^0_{n''}}\right), \tag{e}$$

$$-\frac{1}{2}[S^{(1)}, E^{(2)}]_{n'n} = \frac{i}{2}\frac{(E^{(2)}_{n'} - E^{(2)}_{n})H^{(1)}_{n'n}}{(E^0_n - E^0_{n'})}, \tag{f}$$

$$\frac{i}{12}(S^{(1)}H^{(1)}S^{(1)} - S^{(1)}S^{(1)}H^{(1)})_{n'n} =$$

$$-\frac{i}{6}\sum_{n''\neq n}\frac{H^{(1)}_{n'n}H^{(1)}_{nn''}H^{(1)}_{n''n}}{(E^0_n-E^0_{n'})(E^0_n-E^0_{n''})} + \frac{i}{12}\sum_{n''\neq n', n}\frac{H^{(1)}_{n'n''}H^{(1)}_{n''n}(H^{(1)}_{n''n''} - H^{(1)}_{nn})}{(E^0_{n'}-E^0_{n''})(E^0_n-E^0_{n''})}$$

$$+\frac{i}{12}\sum_{n''\neq n, n'}\ \sum_{n'''\neq n, n''}\frac{H^{(1)}_{n'n''}H^{(1)}_{n''n'''}H^{(1)}_{n'''n}}{(E^0_{n'} - E^0_{n''})}\left(\frac{1}{E^0_n - E^0_{n'''}} + \frac{1}{E^0_{n''} - E^0_{n'''}}\right), \tag{g}$$

$$\frac{i}{12}(S^{(1)}H^{(1)}S^{(1)} - H^{(1)}S^{(1)}S^{(1)})_{n'n} =$$

$$+\frac{i}{6}\sum_{n''\neq n'}\frac{H^{(1)}_{n'n''}H^{(1)}_{n''n'}H^{(1)}_{n'n}}{(E^0_n-E^0_{n'})(E^0_{n'}-E^0_{n''})}+\frac{i}{12}\sum_{n''\neq n,n'}\frac{H^{(1)}_{n'n''}H^{(1)}_{n''n}(H^{(1)}_{n''n''}-H^{(1)}_{n'n'})}{(E^0_n-E^0_{n''})(E^0_{n'}-E^0_{n''})}$$

$$+\frac{i}{12}\sum_{n''\neq n,n'}\sum_{n'''\neq n',n''}\frac{H^{(1)}_{n'n'''}H^{(1)}_{n'''n''}H^{(1)}_{n''n}}{(E^0_n-E^0_{n''})}\left(\frac{1}{E^0_{n'}-E^0_{n'''}}+\frac{1}{E^0_{n''}-E^0_{n'''}}\right),\tag{h}$$

$$\frac{i}{12}(S^{(1)}S^{(1)}E^{(1)}-S^{(1)}E^{(1)}S^{(1)})_{n'n}=\frac{i}{12}\sum_{n''\neq n,n'}\frac{H^{(1)}_{n'n''}H^{(1)}_{n''n}(H^{(1)}_{nn}-H^{(1)}_{n''n''})}{(E^0_n-E^0_{n''})(E^0_{n'}-E^0_{n''})},\tag{i}$$

$$\frac{i}{12}(E^{(1)}S^{(1)}S^{(1)}-S^{(1)}E^{(1)}S^{(1)})_{n'n}=\frac{i}{12}\sum_{n''\neq n,n'}\frac{H^{(1)}_{n'n''}H^{(1)}_{n''n}(H^{(1)}_{n'n'}-H^{(1)}_{n''n''})}{(E^0_n-E^0_{n''})(E^0_{n'}-E^0_{n''})}.\tag{j}$$

Combining (a), (b), and (c) with all of the terms just obtained above and dividing equation (36) by $(E^0_n - E^0_{n'})/i$, one obtains the following for $S^{(3)}_{n'n}$:

(cont'd on next page)

$$\frac{S^{(3)}_{n'n}}{i} = \frac{H^{(3)}_{n'n}}{(E^0_n - E^0_{n'})} + \frac{H^{(2)}_{n'n}\,(H^{(1)}_{n'n'} - H^{(1)}_{nn})}{(E^0_n - E^0_{n'})^2} + \frac{H^{(1)}_{n'n}\,(H^{(1)}_{n'n'} - H^{(1)}_{nn})^2}{(E^0_n - E^0_{n'})^3}$$

$$+ \frac{1}{3}\,\frac{H^{(1)}_{n'n}\,(H^{(2)}_{n'n'} - H^{(2)}_{nn})}{(E^0_n - E^0_{n'})^2} + \frac{2}{3}\,\frac{H^{(1)}_{n'n}\,(E^{(2)}_{n'} - E^{(2)}_{n})}{(E^0_n - E^0_{n'})^2}$$

$$+ \frac{1}{2} \sum_{n''\neq n,\, n'} \left[\left\{ \frac{H^{(1)}_{n'n''}\, H^{(1)}_{n''n}}{(E^0_n - E^0_{n'})} \left(\frac{H^{(1)}_{n''n''} - H^{(1)}_{n'n'}}{(E^0_{n'} - E^0_{n''})^2} + \frac{H^{(1)}_{n''n''} - H^{(1)}_{nn}}{(E^0_n - E^0_{n''})^2} \right) \right. \right.$$

$$+ \frac{H^{(1)}_{n'n''}\, H^{(1)}_{n''n}\,(H^{(1)}_{n'n'} - H^{(1)}_{nn})}{(E^0_n - E^0_{n'})^2} \left(\frac{1}{E^0_n - E^0_{n''}} + \frac{1}{E^0_{n'} - E^0_{n''}} \right)$$

$$\left. + \frac{(H^{(1)}_{n'n''}\, H^{(2)}_{n''n} + H^{(2)}_{n'n''}\, H^{(1)}_{n''n}}{(E^0_n - E^0_{n'})} \left(\frac{1}{E^0_n - E^0_{n''}} + \frac{1}{E^0_{n'} - E^0_{n''}} \right) \right\}$$

$$+ \sum_{n'''\neq n,\, n''} \frac{H^{(1)}_{n'n''}\, H^{(1)}_{n''n'''}\, H^{(1)}_{n'''n}}{4(E^0_n - E^0_{n'})\,(E^0_n - E^0_{n''})} \left(\frac{1}{E^0_n - E^0_{n'''}} + \frac{1}{E^0_{n''} - E^0_{n'''}} \right)$$

$$+ \sum_{n'''\neq n',\, n''} \frac{H^{(1)}_{n'n'''}\, H^{(1)}_{n'''n''}\, H^{(1)}_{n''n}}{4(E^0_n - E^0_{n'})\,(E^0_{n'} - E^0_{n''})} \left(\frac{1}{E^0_{n'} - E^0_{n'''}} + \frac{1}{E^0_{n''} - E^0_{n'''}} \right)$$

$$+ \sum_{n'''\neq n,\, n''} \frac{H^{(1)}_{n'n''}\, H^{(1)}_{n''n'''}\, H^{(1)}_{n'''n}}{12(E^0_n - E^0_{n'})\,(E^0_{n'} - E^0_{n''})} \left(\frac{1}{E^0_n - E^0_{n'''}} + \frac{1}{E^0_{n''} - E^0_{n'''}} \right)$$

$$+ \sum_{n'''\neq n',\, n''} \frac{H^{(1)}_{n'n'''}\, H^{(1)}_{n'''n''}\, H^{(1)}_{n''n}}{12(E^0_n - E^0_{n'})\,(E^0_n - E^0_{n''})} \left(\frac{1}{E^0_{n'} - E^0_{n'''}} + \frac{1}{E^0_{n''} - E^0_{n'''}} \right)$$

A few comments are necessary in regard to the above result. Terms (i) and (j) were cancelled by the middle terms of (g) and (h). By expressing the first terms of (g) and (h) in terms of $E_n^{(2)}$, one can combine them with the second term in (d) and the single term in (f). The last modification is accomplished by taking the first terms in (g) and (h) and expressing them as follows:

By taking

$$\frac{i}{6} \sum_{n''\neq n'} \frac{H^{(1)}_{n'n''} H^{(1)}_{n''n'}}{(E^0_{n'} - E^0_{n''})} \left(\frac{H^{(1)}_{n'n}}{E^0_n - E^0_{n'}} \right) - \frac{i}{6} \frac{H^{(1)}_{n'n}}{(E^0_n - E^0_{n'})} \sum_{n''\neq n} \frac{H^{(1)}_{nn''} H^{(1)}_{n''n}}{(E^0_n - E^0_{n''})} ,$$

then using

$$E^{(2)}_n = H^{(2)}_{nn} + \sum_{n''\neq n} \frac{H^{(1)}_{nn''} H^{(1)}_{n''n}}{(E^0_n - E^0_{n''})} ,$$

one obtains

$$\frac{i}{6} \frac{H^{(1)}_{n'n} (E^{(2)}_{n'} - E^{(2)}_n)}{(E^0_n - E^0_{n'})} - \frac{i}{6} \frac{H^{(1)}_{n'n} (H^{(2)}_{n'n'} - H^{(2)}_{nn})}{(E^0_n - E^0_{n'})} .$$

These terms combine with (f) and the second term in (d), respectively.

With the expression for $S^{(3)}_{n'n}$ established, equation (35) is now evaluated. The same procedure is followed; that is, each term is evaluated separately and then combined to form $E^{(4)}_n$. Going back to equation (35), one notes that the first term to be evaluated is $[S^{(3)}, H^{(1)}]_{nn}$. Using the expression just obtained for $S^{(3)}_{n'n}$, one obtains the following:

$$\frac{i}{2} [S^{(3)}, H^{(1)}]_{nn} \equiv \frac{1}{2} \sum_{n'\neq n} \left\{ H^{(1)}_{nn'} \left(\frac{S^{(3)}_{n'n}}{i} \right) - \left(\frac{S^{(3)}_{nn'}}{i} \right) H^{(1)}_{n'n} \right\}$$

$$
= \sum_{n' \neq n} \Bigg\{ \Bigg(\frac{(H^{(1)}_{nn'} H^{(3)}_{n'n} + H^{(3)}_{nn'} H^{(1)}_{n'n})}{2\,(E^0_n - E^0_{n'})} + \frac{H^{(1)}_{nn'} H^{(2)}_{n'n} (H^{(1)}_{n'n'} - H^{(1)}_{nn})}{2\,(E^0_n - E^0_{n'})^2}
$$

$$
- \frac{H^{(2)}_{nn'} H^{(1)}_{n'n} (H^{(1)}_{nn} - H^{(1)}_{n'n'})}{2\,(E^0_n - E^0_{n'})^2} + \frac{H^{(1)}_{nn'} H^{(1)}_{n'n} (H^{(1)}_{n'n'} - H^{(1)}_{nn})^2}{2\,(E^0_n - E^0_{n'})^3}
$$

$$
- \frac{H^{(1)}_{nn'} H^{(1)}_{n'n} (H^{(1)}_{nn} - H^{(1)}_{n'n'})^2}{2\,(E^0_{n'} - E^0_{n})^3} + \frac{1}{6} \frac{H^{(1)}_{nn'} H^{(1)}_{n'n} (H^{(2)}_{n'n'} - H^{(2)}_{nn})}{(E^0_n - E^0_{n'})^2}
$$

$$
- \frac{1}{6} \frac{H^{(1)}_{nn'} H^{(1)}_{n'n} (H^{(2)}_{nn} - H^{(2)}_{n'n'})}{(E^0_n - E^0_{n'})^2} + \frac{2}{6} \frac{H^{(1)}_{nn'} H^{(1)}_{n'n} (E^{(2)}_{n'} - E^{(2)}_{n})}{(E^0_n - E^0_{n'})^2}
$$

$$
- \frac{2}{6} \frac{H^{(1)}_{nn'} H^{(1)}_{n'n} (E^{(2)}_{n} - E^{(2)}_{n'})}{(E^0_n - E^0_{n'})^2} \Bigg)
$$

$$
+ \sum_{n'' \neq n, n'} \Bigg[\frac{H^{(1)}_{nn'} H^{(1)}_{n'n''} H^{(1)}_{n''n}}{4(E^0_n - E^0_{n'})} \left(\frac{H^{(1)}_{n''n''} - H^{(1)}_{n'n'}}{(E^0_{n'} - E^0_{n''})^2} + \frac{H^{(1)}_{n''n''} - H^{(1)}_{nn}}{(E^0_{n} - E^0_{n''})^2} \right)
$$

$$
+ \frac{H^{(1)}_{nn''} H^{(1)}_{n''n'} H^{(1)}_{n'n}}{4\,(E^0_n - E^0_{n'})} \left(\frac{H^{(1)}_{n''n''} - H^{(1)}_{nn}}{(E^0_{n} - E^0_{n''})^2} + \frac{H^{(1)}_{n''n''} - H^{(1)}_{n'n'}}{(E^0_{n'} - E^0_{n''})^2} \right)
$$

$$
+ \frac{H^{(1)}_{nn'} H^{(1)}_{n'n''} H^{(1)}_{n''n} (H^{(1)}_{n'n'} - H^{(1)}_{nn})}{4\,(E^0_n - E^0_{n'})^2} \left(\frac{1}{E^0_n - E^0_{n''}} + \frac{1}{E^0_{n'} - E^0_{n''}} \right)
$$

$$
+ \frac{H^{(1)}_{nn''} H^{(1)}_{n''n'} H^{(1)}_{n'n} (H^{(1)}_{n'n'} - H^{(1)}_{nn})}{4\,(E^0_n - E^0_{n'})^2} \left(\frac{1}{E^0_n - E^0_{n''}} + \frac{1}{E^0_{n'} - E^0_{n''}} \right)
$$

$$+ \frac{\left(H^{(1)}_{nn'} H^{(1)}_{n'n''} H^{(2)}_{n''n} + H^{(1)}_{nn'} H^{(2)}_{n'n''} H^{(1)}_{n''n}\right)}{4\,(E^0_n - E^0_{n'})} \left(\frac{1}{E^0_n - E^0_{n''}} + \frac{1}{E^0_{n'} - E^0_{n''}} \right)$$

$$+ \frac{\left(H^{(1)}_{nn''} H^{(2)}_{n''n'} H^{(1)}_{n'n} + H^{(2)}_{nn''} H^{(1)}_{n''n'} H^{(1)}_{n'n}\right)}{4\,(E^0_n - E^0_{n'})} \left(\frac{1}{E^0_n - E^0_{n''}} + \frac{1}{E^0_{n'} - E^0_{n''}} \right)$$

$$+ \sum_{n''' \neq n,\, n''} \frac{H^{(1)}_{nn'} H^{(1)}_{n'n''} H^{(1)}_{n''n'''} H^{(1)}_{n'''n}}{8\,(E^0_n - E^0_{n'})\,(E^0_n - E^0_{n''})} \left(\frac{1}{E^0_n - E^0_{n'''}} + \frac{1}{E^0_{n''} - E^0_{n'''}} \right)$$

$$+ \sum_{n''' \neq n',\, n''} \frac{H^{(1)}_{nn''} H^{(1)}_{n''n'''} H^{(1)}_{n'''n'} H^{(1)}_{n'n}}{8\,(E^0_n - E^0_{n'})\,(E^0_{n'} - E^0_{n''})} \left(\frac{1}{E^0_{n'} - E^0_{n'''}} + \frac{1}{E^0_{n''} - E^0_{n'''}} \right)$$

$$+ \sum_{n''' \neq n',\, n''} \frac{H^{(1)}_{nn'} H^{(1)}_{n'n'''} H^{(1)}_{n'''n''} H^{(1)}_{n''n}}{8\,(E^0_n - E^0_{n'})\,(E^0_{n'} - E^0_{n''})} \left(\frac{1}{E^0_{n'} - E^0_{n'''}} + \frac{1}{E^0_{n''} - E^0_{n'''}} \right)$$

$$+ \sum_{n''' \neq n,\, n''} \frac{H^{(1)}_{nn'''} H^{(1)}_{n'''n''} H^{(1)}_{n''n'} H^{(1)}_{n'n}}{8\,(E^0_n - E^0_{n'})\,(E^0_n - E^0_{n''})} \left(\frac{1}{E^0_n - E^0_{n'''}} + \frac{1}{E^0_{n''} - E^0_{n'''}} \right)$$

$$+ \sum_{n''' \neq n,\, n''} \frac{H^{(1)}_{nn'} H^{(1)}_{n'n''} H^{(1)}_{n''n'''} H^{(1)}_{n'''n}}{24\,(E^0_n - E^0_{n'})\,(E^0_{n'} - E^0_{n''})} \left(\frac{1}{E^0_n - E^0_{n'''}} + \frac{1}{E^0_{n''} - E^0_{n'''}} \right)$$

$$+ \sum_{n''' \neq n',\, n''} \frac{H^{(1)}_{nn''} H^{(1)}_{n''n'''} H^{(1)}_{n'''n'} H^{(1)}_{n'n}}{24\,(E^0_n - E^0_{n'})\,(E^0_n - E^0_{n''})} \left(\frac{1}{E^0_{n'} - E^0_{n'''}} + \frac{1}{E^0_{n''} - E^0_{n'''}} \right)$$

$$+ \sum_{n''' \neq n',\, n''} \frac{H^{(1)}_{nn'} H^{(1)}_{n'n'''} H^{(1)}_{n'''n''} H^{(1)}_{n''n}}{24\,(E^0_n - E^0_{n'})\,(E^0_n - E^0_{n''})} \left(\frac{1}{E^0_{n'} - E^0_{n'''}} + \frac{1}{E^0_{n''} - E^0_{n'''}} \right)$$

$$+ \sum_{n'''\neq n, n''} \frac{H^{(1)}_{nn'''} H^{(1)}_{n'''n''} H^{(1)}_{n''n'} H^{(1)}_{n'n}}{24(E^0_n - E^0_{n'})(E^0_{n'} - E^0_{n''})} \left(\frac{1}{E^0_n - E^0_{n'''}} + \frac{1}{E^0_{n''} - E^0_{n'''}} \right) \Bigg] \Bigg] \Bigg\}$$

The range on n''' is not the same on all of the above terms. For this reason the terms containing n''' are not fully combined at this point. Without making additional simplifications, it is helpful to rearrange the above term as follows:

$$\frac{i}{2} [S^{(3)}, H^{(1)}]_{nn} =$$

$$\sum_{n'\neq n} \Bigg\{ \Bigg(\frac{H^{(1)}_{nn'} H^{(3)}_{n'n} + H^{(3)}_{nn'} H^{(1)}_{n'n}}{2(E^0_n - E^0_{n'})} + \frac{H^{(1)}_{nn'} H^{(1)}_{n'n} (H^{(1)}_{n'n'} - H^{(1)}_{nn})^2}{(E^0_n - E^0_{n'})^3}$$

$$+ \frac{H^{(1)}_{nn'} H^{(1)}_{n'n} (H^{(2)}_{n'n'} - H^{(2)}_{nn})}{3(E^0_n - E^0_{n'})^2} + \frac{2}{3} \frac{H^{(1)}_{nn'} H^{(1)}_{n'n} (E^{(2)}_{n'} - E^{(2)}_n)}{(E^0_n - E^0_{n'})^2}$$

$$+ \frac{(H^{(1)}_{nn'} H^{(2)}_{n'n} + H^{(2)}_{nn'} H^{(1)}_{n'n}) (H^{(1)}_{n'n'} - H^{(1)}_{nn})}{(E^0_n - E^0_{n'})^2} \Bigg)$$

$$+ \sum_{n''\neq n, n'} \Bigg[\frac{(H^{(1)}_{nn'} H^{(1)}_{n'n''} H^{(1)}_{n''n} + H^{(1)}_{nn''} H^{(1)}_{n''n'} H^{(1)}_{n'n}) (H^{(1)}_{n'n'} - H^{(1)}_{nn})}{2(E^0_n - E^0_{n'})^2 (E^0_n - E^0_{n''})}$$

$$+ \frac{(H^{(1)}_{nn'} H^{(1)}_{n'n''} H^{(1)}_{n''n} + H^{(1)}_{nn''} H^{(1)}_{n''n'} H^{(1)}_{n'n}) (H^{(1)}_{n'n'} - H^{(1)}_{nn})}{4 (E^0_n - E^0_{n'})^2 (E^0_{n'} - E^0_{n''})}$$

$$+ \frac{(H^{(1)}_{nn'} H^{(1)}_{n'n''} H^{(1)}_{n''n} + H^{(1)}_{nn''} H^{(1)}_{n''n'} H^{(1)}_{n'n}) (H^{(1)}_{n''n''} - H^{(1)}_{n'n'})}{4 (E^0_{n'} - E^0_{n''})^2 (E^0_n - E^0_{n'})}$$

$$+ \frac{(H^{(1)}_{nn'} H^{(1)}_{n'n''} H^{(2)}_{n''n} + H^{(2)}_{nn''} H^{(1)}_{n''n'} H^{(1)}_{n'n})}{4\,(E^0_n - E^0_{n'})} \left(\frac{1}{E^0_n - E^0_{n''}} + \frac{1}{E^0_{n'} - E^0_{n''}} \right)$$

$$+ \frac{(H^{(1)}_{nn'} H^{(2)}_{n'n''} H^{(1)}_{n''n} + H^{(1)}_{nn''} H^{(2)}_{n''n'} H^{(1)}_{n'n})}{4\,(E^0_n - E^0_{n'})} \left(\frac{1}{E^0_n - E^0_{n''}} + \frac{1}{E^0_{n'} - E^0_{n''}} \right)$$

$$+ \sum_{n''' \neq n, n''} \left\{ \frac{(H^{(1)}_{nn'} H^{(1)}_{n'n''} H^{(1)}_{n''n'''} H^{(1)}_{n'''n} + H^{(1)}_{nn'''} H^{(1)}_{n'''n''} H^{(1)}_{n''n'} H^{(1)}_{n'n})}{8\,(E^0_n - E^0_{n'})\,(E^0_n - E^0_{n''})} \right.$$

$$\times \left(\frac{1}{E^0_n - E^0_{n'''}} + \frac{1}{E^0_{n''} - E^0_{n'''}} \right)$$

$$+ \frac{(H^{(1)}_{nn'} H^{(1)}_{n'n''} H^{(1)}_{n''n'''} H^{(1)}_{n'''n} + H^{(1)}_{nn'''} H^{(1)}_{n'''n''} H^{(1)}_{n''n'} H^{(1)}_{n'n})}{24\,(E^0_n - E^0_{n'})\,(E^0_{n'} - E^0_{n''})}$$

$$\left. \times \left(\frac{1}{E^0_n - E^0_{n'''}} + \frac{1}{E^0_{n''} - E^0_{n'''}} \right) \right\}$$

$$+ \sum_{n''' \neq n', n''} \left\{ \frac{(H^{(1)}_{nn''} H^{(1)}_{n''n'''} H^{(1)}_{n'''n'} H^{(1)}_{n'n} + H^{(1)}_{nn'} H^{(1)}_{n'n'''} H^{(1)}_{n'''n''} H^{(1)}_{n''n})}{8\,(E^0_n - E^0_{n'})\,(E^0_{n'} - E^0_{n''})} \right.$$

$$\times \left(\frac{1}{E^0_{n'} - E^0_{n'''}} + \frac{1}{E^0_{n''} - E^0_{n'''}} \right)$$

$$+\frac{(H^{(1)}_{nn''} H^{(1)}_{n''n'''} H^{(1)}_{n'''n'} H^{(1)}_{n'n} + H^{(1)}_{nn'} H^{(1)}_{n'n'''} H^{(1)}_{n'''n''} H^{(1)}_{n''n})}{24\ (E^0_n - E^0_{n'})\ (E^0_n - E^0_{n''})}$$

$$\left.\left.\left.\times \left(\frac{1}{E^0_{n'} - E^0_{n'''}} + \frac{1}{E^0_{n''} - E^0_{n'''}} \right)\right\}\right]\right\}$$

The above term is the longest and most important in $E_n^{(4)}$. The remaining terms are obtained as a group below. Omitting intermediate steps, these terms are:

$$\frac{i}{2}\,[S^{(2)}, H^{(2)}]_{nn} = \sum_{n'\neq n}\left[\left\{\frac{H^{(2)}_{nn'} H^{(2)}_{n'n}}{(E^0_n - E^0_{n'})} + \frac{1}{2}\,\frac{(H^{(1)}_{nn'} H^{(2)}_{n'n} + H^{(2)}_{nn'} H^{(1)}_{n'n})(H^{(1)}_{n'n'} - H^{(1)}_{nn})}{(E^0_n - E^0_{n'})^2}\right\}\right.$$

$$\left.+\frac{1}{4}\sum_{n'\neq n}\ \sum_{n''\neq n, n'} \frac{(H^{(1)}_{nn''} H^{(1)}_{n''n'} H^{(2)}_{n'n} + H^{(2)}_{nn'} H^{(1)}_{n'n''} H^{(1)}_{n''n})}{(E^0_n - E^0_{n'})} \left(\frac{1}{E^0_n - E^0_{n''}} + \frac{1}{E^0_{n'} - E^0_{n''}} \right)\right] \qquad (\alpha)$$

$$\frac{i}{2}\,[S^{(1)}, H^{(3)}]_{nn} = \frac{1}{2}\sum_{n'\neq n} \frac{(H^{(1)}_{nn'} H^{(3)}_{n'n} + H^{(3)}_{nn'} H^{(1)}_{n'n})}{(E^0_n - E^0_{n'})}, \qquad (\beta)$$

$$\frac{1}{12}\,(S^{(1)} H^{(2)} S^{(1)} + S^{(1)} H^{(2)} S^{(1)})_{nn} = \frac{1}{6}\sum_{n'\neq n} \frac{(H^{(1)}_{nn'} H^{(1)}_{n'n})\, H^{(2)}_{n'n'}}{(E^0_n - E^0_{n'})^2}$$

$$+\frac{1}{12}\sum_{n'\neq n}\ \sum_{n''\neq n, n'} \frac{(H^{(1)}_{nn'} H^{(2)}_{n'n''} H^{(1)}_{n''n} + H^{(1)}_{nn''} H^{(2)}_{n''n'} H^{(1)}_{n'n})}{(E^0_n - E^0_{n'})\ (E^0_n - E^0_{n''})}, \qquad (\gamma)$$

$$-\frac{1}{12}\,(H^{(2)} S^{(1)} S^{(1)} + S^{(1)} S^{(1)} H^{(2)})_{nn} = -\frac{1}{6}\sum_{n'\neq n} \frac{(H^{(1)}_{nn'} H^{(1)}_{n'n})\, H^{(2)}_{nn}}{(E^0_n - E^0_{n'})^2}$$

$$+\frac{1}{12}\sum_{n'\neq n}\;\sum_{n''\neq n, n'}\frac{(H^{(2)}_{nn''}\,H^{(1)}_{n''n'}\,H^{(1)}_{n'n}+H^{(1)}_{nn'}\,H^{(1)}_{n'n''}\,H^{(2)}_{n''n})}{(E^0_n-E^0_{n'})\,(E^0_{n'}-E^0_{n''})}, \qquad (\delta)$$

$$\frac{1}{12}\,(S^{(1)}\,S^{(1)}\,E^{(2)}-S^{(1)}\,E^{(2)}\,S^{(1)})_{nn}=\frac{1}{12}\sum_{n'\neq n}\frac{H^{(1)}_{nn'}\,H^{(1)}_{n'n}\,(E^{(2)}_n-E^{(2)}_{n'})}{(E^0_n-E^0_{n'})^2}, \qquad (\epsilon)$$

$$\frac{1}{12}\,(E^{(2)}\,S^{(1)}\,S^{(1)}-S^{(1)}\,E^{(2)}\,S^{(1)})_{nn}=\frac{1}{12}\sum_{n'\neq n}\frac{H^{(1)}_{nn'}\,H^{(1)}_{n'n}\,(E^{(2)}_n-E^{(2)}_{n'})}{(E^0_n-E^0_{n'})^2}, \qquad (\zeta)$$

(The next two terms are equal)

$$\frac{2}{12}\,(S^{(2)}\,H^{(1)}\,S^{(1)}+S^{(1)}\,H^{(1)}\,S^{(2)})_{nn}=$$

$$\sum_{n'\neq n}\left[\frac{2}{12}\,\frac{(H^{(2)}_{nn'}\,H^{(1)}_{n'n}+H^{(1)}_{nn'}\,H^{(2)}_{n'n})\,H^{(1)}_{n'n'}}{(E^0_n-E^0_{n'})^2}+\frac{4}{12}\,\frac{H^{(1)}_{nn'}\,H^{(1)}_{n'n}\,(H^{(1)}_{n'n'}-H^{(1)}_{nn})\,H^{(1)}_{n'n'}}{(E^0_n-E^0_{n'})^3}\right.$$

$$+\sum_{n''\neq n, n'}\left\{\frac{2}{12}\,\frac{(H^{(2)}_{nn'}\,H^{(1)}_{n'n''}\,H^{(1)}_{n''n}+H^{(1)}_{nn''}\,H^{(1)}_{n''n'}\,H^{(2)}_{n'n})}{(E^0_n-E^0_{n'})\,(E^0_n-E^0_{n''})}\right.$$

$$+\frac{2}{12}\,\frac{(H^{(1)}_{nn'}\,H^{(1)}_{n'n''}\,H^{(1)}_{n''n}+H^{(1)}_{nn''}\,H^{(1)}_{n''n'}\,H^{(1)}_{n'n})\,(H^{(1)}_{n'n'}-H^{(1)}_{nn})}{(E^0_n-E^0_{n'})^2\,(E^0_n-E^0_{n''})}$$

$$+\frac{2}{24}\,\frac{(H^{(1)}_{nn''}\,H^{(1)}_{n''n'}\,H^{(1)}_{n'n}+H^{(1)}_{nn'}\,H^{(1)}_{n'n''}\,H^{(1)}_{n''n})\,H^{(1)}_{n'n'}}{(E^0_n-E^0_{n'})^2}$$

$$\times\left(\frac{1}{E^0_n-E^0_{n''}}+\frac{1}{E^0_{n'}-E^0_{n''}}\right)$$

$$+\frac{2}{24}\sum_{n'''\neq n,n''}\frac{(H^{(1)}_{nn'''}H^{(1)}_{n'''n''}H^{(1)}_{n''n'}H^{(1)}_{n'n}+H^{(1)}_{nn'}H^{(1)}_{n'n''}H^{(1)}_{n''n'''}H^{(1)}_{n'''n})}{(E^0_n-E^0_{n'})(E^0_n-E^0_{n''})}$$

$$\times\left(\frac{1}{E^0_n-E^0_{n'''}}+\frac{1}{E^0_{n''}-E^0_{n'''}}\right)\Bigg\}\Bigg]\quad(\eta)$$

$$-\frac{1}{12}(H^{(1)}S^{(1)}S^{(2)}+S^{(2)}S^{(1)}H^{(1)})_{nn}=$$

$$\sum_{n'\neq n}\Bigg[-\frac{1}{12}\frac{(H^{(1)}_{nn'}H^{(2)}_{n'n}+H^{(2)}_{nn'}H^{(1)}_{n'n})H^{(1)}_{nn}}{(E^0_n-E^0_{n'})^2}-\frac{2}{12}\frac{H^{(1)}_{nn'}H^{(1)}_{n'n}(H^{(1)}_{n'n'}-H^{(1)}_{nn})H^{(1)}_{nn}}{(E^0_n-E^0_{n'})^3}$$

$$+\sum_{n''\neq n,n'}\Bigg\{\frac{1}{12}\frac{H^{(1)}_{nn''}H^{(1)}_{n''n'}H^{(2)}_{n'n}+H^{(2)}_{nn'}H^{(1)}_{n'n''}H^{(1)}_{n''n})}{(E^0_n-E^0_{n'})(E^0_{n'}-E^0_{n''})}$$

$$+\frac{1}{12}\frac{(H^{(1)}_{nn''}H^{(1)}_{n''n'}H^{(1)}_{n'n}+H^{(1)}_{nn'}H^{(1)}_{n'n''}H^{(1)}_{n''n})(H^{(1)}_{n'n'}-H^{(1)}_{nn})}{(E^0_n-E^0_{n'})^2(E^0_{n'}-E^0_{n''})}$$

$$-\frac{1}{24}\frac{(H^{(1)}_{nn'}H^{(1)}_{n'n''}H^{(1)}_{n''n}+H^{(1)}_{nn''}H^{(1)}_{n''n'}H^{(1)}_{n'n})H^{(1)}_{nn}}{(E^0_n-E^0_{n'})^2}$$

$$\times\left(\frac{1}{E^0_n-E^0_{n''}}+\frac{1}{E^0_{n'}-E^0_{n''}}\right)$$

$$+\frac{1}{24}\sum_{n'''\neq n,n'}\frac{(H^{(1)}_{nn''}H^{(1)}_{n''n'}H^{(1)}_{n'n'''}H^{(1)}_{n'''n}+H^{(1)}_{nn'''}H^{(1)}_{n'''n'}H^{(1)}_{n'n''}H^{(1)}_{n''n})}{(E^0_n-E^0_{n'})\,(E^0_{n'}-E^0_{n''})}$$

$$\times\left(\frac{1}{E^0_n-E^0_{n'''}}+\frac{1}{E^0_{n'}-E^0_{n'''}}\right)\Bigg\}\Bigg], \quad (\theta)$$

$$-\frac{1}{12}(S^{(1)}\,S^{(2)}\,H^{(1)}+H^{(1)}\,S^{(2)}\,S^{(1)})_{nn}=$$

$$\sum_{n'\neq n}\Bigg[\Bigg(-\frac{1}{12}\frac{(H^{(2)}_{nn'}H^{(1)}_{n'n}+H^{(1)}_{nn'}H^{(2)}_{n'n})\,H^{(1)}_{nn}}{(E^0_n-E^0_{n'})^2}-\frac{2}{12}\frac{H^{(1)}_{nn'}H^{(1)}_{n'n}\,(H^{(1)}_{n'n'}-H^{(1)}_{nn})\,H^{(1)}_{nn}}{(E^0_n-E^0_{n'})^3}\Bigg)$$

$$+\sum_{n''\neq n,n'}\Bigg[\Bigg(\frac{1}{12}\frac{(H^{(1)}_{nn''}H^{(2)}_{n''n'}H^{(1)}_{n'n}+H^{(1)}_{nn'}H^{(2)}_{n'n''}H^{(1)}_{n''n})}{(E^0_n-E^0_{n'})\,(E^0_{n'}-E^0_{n''})}$$

$$+\frac{1}{12}\frac{(H^{(1)}_{nn'}H^{(1)}_{n'n''}H^{(1)}_{n''n}+H^{(1)}_{nn''}H^{(1)}_{n''n'}H^{(1)}_{n'n})\,(H^{(1)}_{n''n''}-H^{(1)}_{n'n'})}{(E^0_n-E^0_{n'})\,(E^0_{n'}-E^0_{n''})^2}\Bigg)$$

$$-\frac{1}{24}\frac{(H^{(1)}_{nn'}H^{(1)}_{n'n''}H^{(1)}_{n''n}+H^{(1)}_{nn''}H^{(1)}_{n''n'}H^{(1)}_{n'n})\,H^{(1)}_{nn}}{(E^0_n-E^0_{n'})^2}$$

$$\times\left(\frac{1}{E^0_{n'}-E^0_{n''}}+\frac{1}{E^0_n-E^0_{n''}}\right)$$

$$+\frac{1}{24}\sum_{n'''\neq n',n''}\frac{(H^{(1)}_{nn'}H^{(1)}_{n'n'''}H^{(1)}_{n'''n''}H^{(1)}_{n''n}+H^{(1)}_{nn''}H^{(1)}_{n''n'''}H^{(1)}_{n'''n'}H^{(1)}_{n'n})}{(E^0_n-E^0_{n'})\,(E^0_{n'}-E^0_{n''})}$$

$$\times\left(\frac{1}{E^0_{n'}-E^0_{n'''}}+\frac{1}{E^0_{n''}-E^0_{n'''}}\right)\Bigg\}\Bigg], \quad (\iota)$$

$$\frac{1}{12}\left(S^{(2)}\, S^{(1)}\, E^{(1)} + E^{(1)}\, S^{(1)}\, S^{(2)}\right)_{nn} =$$

$$\sum_{n'\neq n}\Bigg[\frac{1}{12}\,\frac{\left(H^{(2)}_{nn'}\, H^{(1)}_{n'n} + H^{(1)}_{nn'}\, H^{(2)}_{n'n}\right) H^{(1)}_{nn}}{\left(E^0_n - E^0_{n'}\right)^2} + \frac{1}{6}\,\frac{H^{(1)}_{nn'}\, H^{(1)}_{n'n}\left(H^{(1)}_{n'n'} - H^{(1)}_{nn}\right) H^{(1)}_{nn}}{\left(E^0_n - E^0_{n'}\right)^3}$$

$$\frac{1}{24}\sum_{n''\neq n,\, n'}\frac{\left(H^{(1)}_{nn''}\, H^{(1)}_{n''n'}\, H^{(1)}_{n'n} + H^{(1)}_{nn'}\, H^{(1)}_{n'n''}\, H^{(1)}_{n''n}\right) H^{(1)}_{nn}}{\left(E^0_n - E^0_{n'}\right)^2}$$

$$\times\left(\frac{1}{E^0_n - E^0_{n''}} + \frac{1}{E^0_{n'} - E^0_{n''}}\right)\Bigg] \qquad (\kappa)$$

$$\frac{1}{12}\left(E^{(1)}\, S^{(2)}\, S^{(1)} + S^{(1)}\, S^{(2)}\, E^{(1)}\right)_{nn} =$$

$$\sum_{n'\neq n}\Bigg[\frac{1}{12}\,\frac{\left(H^{(2)}_{nn'}\, H^{(1)}_{n'n} + H^{(1)}_{nn'}\, H^{(2)}_{n'n}\right) H^{(1)}_{nn}}{\left(E^0_n - E^0_{n'}\right)^2} + \frac{1}{6}\,\frac{H^{(1)}_{nn'}\, H^{(1)}_{n'n}\left(H^{(1)}_{n'n'} - H^{(1)}_{nn}\right) H^{(1)}_{nn}}{\left(E^0_n - E^0_{n'}\right)^3}$$

$$+\frac{1}{24}\sum_{n''\neq n,\, n'}\frac{\left(H^{(1)}_{nn'}\, H^{(1)}_{n'n''}\, H^{(1)}_{n''n} + H^{(1)}_{nn''}\, H^{(1)}_{n''n'}\, H^{(1)}_{n'n}\right) H^{(1)}_{nn}}{\left(E^0_n - E^0_{n'}\right)^2}$$

$$\times\left(\frac{1}{E^0_n - E^0_{n''}} + \frac{1}{E^0_{n'} - E^0_{n''}}\right)\Bigg], \qquad (\lambda)$$

(The last two terms yield the same results.) The next two terms are identical;

$$-\frac{2}{12}\left(S^{(1)}\, E^{(1)}\, S^{(2)} + S^{(2)}\, E^{(1)}\, S^{(1)}\right)_{nn} =$$

$$\sum_{n'\neq n}\Bigg[-\frac{2}{12}\,\frac{\left(H^{(2)}_{nn'}\, H^{(1)}_{n'n} + H^{(1)}_{nn'}\, H^{(2)}_{n'n}\right) H^{(1)}_{n'n'}}{\left(E^0_n - E^0_{n'}\right)^2} - \frac{2}{6}\,\frac{H^{(1)}_{nn'}\, H^{(1)}_{n'n}\left(H^{(1)}_{n'n'} - H^{(1)}_{nn}\right) H^{(1)}_{n'n'}}{\left(E^0_n - E^0_{n'}\right)^3}$$

$$-\frac{2}{24}\sum_{n''\neq n,n'}\frac{(H^{(1)}_{nn''}H^{(1)}_{n''n'}H^{(1)}_{n'n}+H^{(1)}_{nn'}H^{(1)}_{n'n''}H^{(1)}_{n''n})}{(E^0_n-E^0_{n'})^2}\left(\frac{1}{E^0_n-E^0_{n''}}+\frac{1}{E^0_{n'}-E^0_{n''}}\right)\Bigg]\Bigg](\mu)$$

To simplify the algebra, the above terms just obtained (α, $\beta,\gamma,\ldots$) are combined separately before they are added to $H^{(4)}_{nn}$ and $[S^{(3)}, H^{(1)}]$. Taking terms α, β, $\gamma,\ldots$ one obtains the following expression:

$$\sum_{n'\neq n}\Bigg[\Bigg(\frac{(H^{(1)}_{nn'}H^{(3)}_{n'n}+H^{(3)}_{nn'}H^{(1)}_{n'n})}{2\,(E^0_n-E^0_{n'})}+\frac{H^{(2)}_{nn'}H^{(2)}_{n'n}}{(E^0_n-E^0_{n'})}$$

$$+\frac{H^{(1)}_{nn'}H^{(1)}_{n'n}(H^{(2)}_{n'n'}-H^{(2)}_{nn})}{6\,(E^0_n-E^0_{n'})^2}-\frac{H^{(1)}_{nn'}H^{(1)}_{n'n}(E^{(2)}_{n'}-E^{(2)}_{n})}{6\,(E^0_n-E^0_{n'})^2}$$

$$+\frac{(H^{(1)}_{nn'}H^{(2)}_{n'n}+H^{(2)}_{nn'}H^{(1)}_{n'n})(H^{(1)}_{n'n'}-H^{(1)}_{nn})}{(E^0_n-E^0_{n'})^2}\Bigg)$$

$$+\sum_{n''\neq n,n'}\Bigg\{\frac{(H^{(1)}_{nn''}H^{(1)}_{n''n'}H^{(2)}_{n'n}+H^{(2)}_{nn'}H^{(1)}_{n'n''}H^{(1)}_{n''n})}{3\,(E^0_n-E^0_{n'})}\left(\frac{1}{E^0_n-E^0_{n''}}+\frac{1}{E^0_{n'}-E^0_{n''}}\right)$$

$$+\frac{(H^{(1)}_{nn'}H^{(2)}_{n'n''}H^{(1)}_{n''n}+H^{(1)}_{nn''}H^{(2)}_{n''n'}H^{(1)}_{n'n})}{12\,(E^0_n-E^0_{n'})}\left(\frac{1}{E^0_n-E^0_{n''}}+\frac{1}{E^0_{n'}-E^0_{n''}}\right)$$

$$+\frac{(H^{(2)}_{nn''}H^{(1)}_{n''n'}H^{(1)}_{n'n}+H^{(1)}_{nn'}H^{(1)}_{n'n''}H^{(2)}_{n''n})}{12\,(E^0_n-E^0_{n'})}\left(\frac{1}{E^0_n-E^0_{n''}}+\frac{1}{E^0_{n'}-E^0_{n''}}\right)$$

$$+\frac{(H^{(1)}_{nn'}H^{(1)}_{n'n''}H^{(1)}_{n''n}+H^{(1)}_{nn''}H^{(1)}_{n''n'}H^{(1)}_{n'n})(H^{(1)}_{n'n'}-H^{(1)}_{nn})}{6\,(E^0_n-E^0_{n'})^2(E^0_n-E^0_{n''})}$$

$$+\frac{\left(H^{(1)}_{nn'}\,H^{(1)}_{n'n''}\,H^{(1)}_{n''n}+H^{(1)}_{nn''}\,H^{(1)}_{n''n'}\,H^{(1)}_{n'n}\right)\left(H^{(1)}_{n'n'}-H^{(1)}_{nn}\right)}{12\,(E^0_n-E^0_{n'})^2\,(E^0_{n'}-E^0_{n''})}$$

$$+\frac{\left(H^{(1)}_{nn'}\,H^{(1)}_{n'n''}\,H^{(1)}_{n''n}+H^{(1)}_{nn''}\,H^{(1)}_{n''n'}\,H^{(1)}_{n'n}\right)\left(H^{(1)}_{n''n''}-H^{(1)}_{n'n'}\right)}{12\,(E^0_n-E^0_{n'})\,(E^0_{n'}-E^0_{n''})^2}$$

$$+\sum_{n'''\neq n,n''}\frac{2\left(H^{(1)}_{nn'''}\,H^{(1)}_{n'''n''}\,H^{(1)}_{n''n'}\,H^{(1)}_{n'n}+H^{(1)}_{nn'}\,H^{(1)}_{n'n''}\,H^{(1)}_{n''n'''}\,H^{(1)}_{n'''n}\right)}{24\,(E^0_n-E^0_{n'})\,(E^0_n-E^0_{n''})}$$

$$\times\left(\frac{1}{E^0_n-E^0_{n'''}}+\frac{1}{E^0_{n''}-E^0_{n'''}}\right)$$

$$+\sum_{n'''\neq n,n'}\frac{\left(H^{(1)}_{nn''}\,H^{(1)}_{n''n'}\,H^{(1)}_{n'n'''}\,H^{(1)}_{n'''n}\quad H^{(1)}_{nn'''}\,H^{(1)}_{n'''n'}\,H^{(1)}_{n'n''}\,H^{(1)}_{n''n}\right)}{24\,(E^0_n-E^0_{n'})\,(E^0_{n'}-E^0_{n''})}$$

$$\times\left(\frac{1}{E^0_n-E^0_{n'''}}+\frac{1}{E^0_{n'}-E^0_{n'''}}\right)$$

$$+\sum_{n'''\neq n',n''}\frac{\left(H^{(1)}_{nn'}\,H^{(1)}_{n'n'''}\,H^{(1)}_{n'''n''}\,H^{(1)}_{n''n}+H^{(1)}_{nn''}\,H^{(1)}_{n''n'''}\,H^{(1)}_{n'''n'}\,H^{(1)}_{n'n}\right)}{24\,(E^0_n-E^0_{n'})\,(E^0_{n'}-E^0_{n''})}$$

$$\times\left(\frac{1}{E^0_{n'}-E^0_{n'''}}+\frac{1}{E^0_{n''}-E^0_{n'''}}\right)\Bigg\}\Bigg]$$

Incorporating the above terms with $[S^{(3)}, H^{(1)}]$ and $H^{(4)}_{nn}$ one obtains,

$$E_n^{(4)} = H_{nn}^{(4)} + \sum_{n'\neq n} \left\{ \frac{H_{nn'}^{(2)} H_{n'n}^{(2)}}{(E_n^0 - E_{n'}^0)} + \frac{H_{nn'}^{(1)} H_{n'n}^{(3)} + H_{nn'}^{(3)} H_{n'n}^{(1)}}{(E_n^0 - E_{n'}^0)} \right.$$

$$+ \frac{H_{nn'}^{(1)} H_{n'n}^{(1)} (H_{n'n'}^{(1)} - H_{nn}^{(1)})^2}{(E_n^0 - E_{n'}^0)^3} + \frac{(H_{nn'}^{(1)} H_{n'n}^{(2)} + H_{nn'}^{(2)} H_{n'n}^{(1)})\ (H_{n'n'}^{(1)} - H_{nn}^{(1)})}{(E_n^0 - E_{n'}^0)^2}$$

$$\left. + \frac{H_{nn'}^{(1)} H_{n'n}^{(1)} (E_{n'}^{(2)} - E_n^{(2)})}{2\ (E_n^0 - E_{n'}^0)^2} + \frac{H_{nn'}^{(1)} H_{n'n}^{(1)} (H_{n'n'}^{(2)} - H_{nn}^{(2)})}{2\ (E_n^0 - E_{n'}^0)^2} \right\}$$

$$+ \sum_{n'\neq n} \ \sum_{n''\neq n,\, n'} \left[\left\{ \frac{(H_{nn'}^{(1)} H_{n'n''}^{(1)} H_{n''n}^{(2)} + H_{nn''}^{(2)} H_{n''n'}^{(1)} H_{n'n}^{(1)})}{3\ (E_n^0 - E_{n'}^0)} \right. \right.$$

$$\times \left(\frac{1}{E_n^0 - E_{n''}^0} + \frac{1}{E_{n'}^0 - E_{n''}^0} \right)$$

$$+ \frac{(H_{nn''}^{(1)} H_{n''n'}^{(1)} H_{n'n}^{(2)} + H_{nn'}^{(2)} H_{n'n''}^{(1)} H_{n''n}^{(1)})}{3\ (E_n^0 - E_{n'}^0)} \left(\frac{1}{E_n^0 - E_{n''}^0} + \frac{1}{E_{n'}^0 - E_{n''}^0} \right)$$

$$+ \frac{(H_{nn'}^{(1)} H_{n'n''}^{(2)} H_{n''n}^{(1)} + H_{nn''}^{(1)} H_{n''n'}^{(2)} H_{n'n}^{(1)})}{3\ (E_n^0 - E_{n'}^0)} \left(\frac{1}{E_n^0 - E_{n''}^0} + \frac{1}{E_{n'}^0 - E_{n''}^0} \right)$$

$$+ \frac{2\ (H_{nn'}^{(1)} H_{n'n''}^{(1)} H_{n''n}^{(1)} + H_{nn''}^{(1)} H_{n''n'}^{(1)} H_{n'n}^{(1)})\ (H_{n'n'}^{(1)} - H_{nn}^{(1)})}{3\ (E_n^0 - E_{n'}^0)^2\ (E_n^0 - E_{n''}^0)}$$

$$+ \frac{(H_{nn'}^{(1)} H_{n'n''}^{(1)} H_{n''n}^{(1)} + H_{nn''}^{(1)} H_{n''n'}^{(1)} H_{n'n}^{(1)})\ (H_{n'n'}^{(1)} - H_{nn}^{(1)})}{3\ (E_n^0 - E_{n'}^0)^2\ (E_{n'}^0 - E_{n''}^0)}$$

$$\left. + \frac{(H_{nn'}^{(1)} H_{n'n''}^{(1)} H_{n''n}^{(1)} + H_{nn''}^{(1)} H_{n''n'}^{(1)} H_{n'n}^{(1)})\ (H_{n''n''}^{(1)} - H_{n'n'}^{(1)})}{3\ (E_n^0 - E_{n'}^0)\ (E_{n'}^0 - E_{n''}^0)^2} \right\}$$

$$\sum_{n'''\neq n, n''} \frac{5(H^{(1)}_{nn'} H^{(1)}_{n'n''} H^{(1)}_{n''n'''} H^{(1)}_{n'''n} + H^{(1)}_{nn'''} H^{(1)}_{n'''n''} H^{(1)}_{n''n'} H^{(1)}_{n'n})}{24\ (E^0_n - E^0_{n'})\ (E^0_n - E^0_{n''})}$$

$$\times \left(\frac{1}{E^0_n - E^0_{n'''}} + \frac{1}{E^0_{n''} - E^0_{n'''}}\right)$$

$$\sum_{n'''\neq n', n''} \frac{4(H^{(1)}_{nn''} H^{(1)}_{n''n'''} H^{(1)}_{n'''n'} H^{(1)}_{n'n} + H^{(1)}_{nn'} H^{(1)}_{n'n'''} H^{(1)}_{n'''n''} H^{(1)}_{n''n})}{24\ (E^0_n - E^0_{n'})\ (E^0_{n'} - E^0_{n''})}$$

$$\times \left(\frac{1}{E^0_{n'} - E^0_{n'''}} + \frac{1}{E^0_{n''} - E^0_{n'''}}\right)$$

$$\sum_{n'''\neq n, n''} \frac{(H^{(1)}_{nn'} H^{(1)}_{n'n''} H^{(1)}_{n''n'''} H^{(1)}_{n'''n} + H^{(1)}_{nn'''} H^{(1)}_{n'''n''} H^{(1)}_{n''n'} H^{(1)}_{n'n})}{24\ (E^0_n - E^0_{n'})\ (E^0_{n'} - E^0_{n''})}$$

$$\times \left(\frac{1}{E^0_n - E^0_{n'''}} + \frac{1}{E^0_{n''} - E^0_{n'''}}\right)$$

$$\sum_{n'''\neq n', n''} \frac{(H^{(1)}_{nn''} H^{(1)}_{n''n'''} H^{(1)}_{n'''n'} H^{(1)}_{n'n} + H^{(1)}_{nn'} H^{(1)}_{n'n'''} H^{(1)}_{n'''n''} H^{(1)}_{n''n})}{24\ (E^0_n - E^0_{n'})\ (E^0_n - E^0_{n''})}$$

$$\times \left(\frac{1}{E^0_{n'} - E^0_{n'''}} + \frac{1}{E^0_{n''} - E^0_{n'''}}\right)$$

$$\sum_{n'''\neq n, n'} \frac{(H^{(1)}_{nn''} H^{(1)}_{n''n'} H^{(1)}_{n'n'''} H^{(1)}_{n'''n} + H^{(1)}_{nn'''} H^{(1)}_{n'''n'} H^{(1)}_{n'n''} H^{(1)}_{n''n}}{24\ (E^0_n - E^0_{n'})\ (E^0_{n'} - E^0_{n''})}$$

$$\times \left(\frac{1}{E^0_n - E_{n'''}} + \frac{1}{E^0_{n'} - E^0_{n'''}}\right)\Bigg]$$

If the above result is to be used for numerical calculations, it is necessary to simplify $E_n^{(4)}$ as much as possible. With the exception of the terms containing triple sums, all the terms in $E_n^{(4)}$ can be recombined into a more compact form. The range on n''' may be standarized by removing terms corresponding to n''' = n, n', or n'' where necessary in order to obtain quantities of the form

$$\sum_{n' \neq n} \sum_{n'' \neq n, n'} \sum_{n''' \neq n, n', n''} Q \ldots \quad .$$

Referring to $E_n^{(4)}$, one needs to take out the factor corresponding to n''' = n' in the first triple sum which gives

$$\frac{5}{24} \sum_{n' \neq n} \sum_{n'' \neq n, n'} \frac{(H^{(1)}_{nn'} H^{(1)}_{n'n''} H^{(1)}_{n''n'} H^{(1)}_{n'n})}{(E^0_n - E^0_{n'})(E^0_n - E^0_{n''})} \left(\frac{1}{E^0_n - E^0_{n'}} - \frac{1}{E^0_{n'} - E^0_{n''}} \right) \tag{A}$$

From the second term, one needs to take out the factor corresponding to n''' = n, which gives

$$\frac{4}{24} \sum_{n' \neq n} \sum_{n'' \neq n, n'} \frac{(H^{(1)}_{nn''} H^{(1)}_{n''n} H^{(1)}_{nn'} H^{(1)}_{n'n} + H^{(1)}_{nn'} H^{(1)}_{n'n} H^{(1)}_{nn''} H^{(1)}_{n''n})}{(E^0_n - E^0_{n'})(E^0_{n'} - E^0_{n''})} \times \left(\frac{1}{E^0_{n'} - E^0_n} + \frac{1}{E_{n''} - E_n} \right) .$$

Letting n'' = n' in the second factor, the above reduces to

$$\frac{-4}{24} \sum_{n' \neq n} \sum_{n'' \neq n, n'} \frac{(H^{(1)}_{nn''} H^{(1)}_{n''n} H^{(1)}_{nn'} H^{(1)}_{n'n})}{(E^0_n - E^0_{n''})(E^0_n - E^0_{n'})} \left(\frac{1}{E^0_n - E^0_{n'}} + \frac{1}{E^0_n - E^0_{n''}} \right) \tag{B}$$

From the third term, for n''' = n', one gets

$$\frac{1}{12} \sum_{n' \neq n} \sum_{n'' \neq n, n'} \frac{(H^{(1)}_{nn'} H^{(1)}_{n'n''} H^{(1)}_{n''n'} H^{(1)}_{n'n})}{(E^0_n - E^0_{n'})(E^0_{n'} - E^0_{n''})} \left(\frac{1}{E^0_n - E^0_{n'}} - \frac{1}{E^0_{n'} - E^0_{n''}} \right) \tag{C}$$

From the fourth term, for n''' = n, one obtains

$$-\frac{1}{12} \sum_{n' \neq n} \sum_{n'' \neq n, n'} \frac{(H^{(1)}_{nn''} H^{(1)}_{n''n} H^{(1)}_{nn'} H^{(1)}_{n'n})}{(E^0_n - E^0_{n''})(E^0_n - E^0_{n'})} \left(\frac{1}{E^0_n - E^0_{n'}} + \frac{1}{E^0_n - E^0_{n''}} \right) . \qquad \text{(D)}$$

From the last term, for n''' = n'', one obtains

$$-\frac{1}{12} \sum_{n' \neq n} \sum_{n'' \neq n, n'} \frac{(H^{(1)}_{nn'} H^{(1)}_{n'n''} H^{(1)}_{n''n'} H^{(1)}_{n'n})}{(E^0_n - E^0_{n''})(E^0_{n'} - E^0_{n''})} \left(\frac{1}{E^0_n - E^0_{n'}} - \frac{1}{E^0_{n'} - E^0_{n''}} \right) . \qquad \text{(E)}$$

Combining the above terms, one obtains the following:

From (C) and (E), one gets

$$\frac{1}{12} \sum_{n' \neq n} \sum_{n'' \neq n, n'} \frac{H^{(1)}_{nn'} H^{(1)}_{n'n''} H^{(1)}_{n''n'} H^{(1)}_{n'n}}{(E^0_n - E^0_{n'})(E^0_n - E^0_{n''})} \left(\frac{1}{E^0_n - E^0_{n'}} - \frac{1}{E^0_{n'} - E^0_{n''}} \right) .$$

This, in turn, adds to (A) giving

$$\frac{1}{2} \sum_{n' \neq n} \sum_{n'' \neq n, n'} \frac{(H^{(1)}_{nn'} H^{(1)}_{n'n''} H^{(1)}_{n''n'} H^{(1)}_{n'n})}{(E^0_n - E^0_{n'})(E^0_n - E^0_{n''})} \left(\frac{1}{E^0_n - E^0_{n'}} - \frac{1}{E^0_{n'} - E^0_{n''}} \right) . \qquad \text{(ACE)}$$

Terms (B) and (D) yield

$$-\frac{1}{4} \sum_{n' \neq n} \sum_{n'' \neq n, n'} \frac{(H^{(1)}_{nn''} H^{(1)}_{n''n} H^{(1)}_{nn'} H^{(1)}_{n'n})}{(E^0_n - E^0_{n'})(E^0_n - E^0_{n''})} \left(\frac{1}{E_n - E_{n'}} + \frac{1}{E^0_n - E^0_{n''}} \right) . \qquad \text{(BD)}$$

Terms (ACE) and (BD) must be added to $E^{(4)}_n$ when it is expressed in terms of the newly defined triple sums.

Since the triple sums are now alike in their summation indices, one recombines these terms into a more symmetric form. The most logical arrangement would be to express each one of the terms as matrix products of the form

$$H^{(1)}_{nn'} H^{(1)}_{n'n''} H^{(1)}_{n''n'''} H^{(1)}_{n'''n} .$$

In order to accomplish this, consider the terms in the order in which they appear in $E^{(4)}_n$. Multiplying the first term out and separating the product into four factors, one obtains

$$\frac{5}{24} \sum_{n'\neq n} \sum_{n''\neq n, n'} \sum_{n'''\neq n, n', n''} \left\{ \frac{H^{(1)}_{nn'} H^{(1)}_{n'n''} H^{(1)}_{n''n'''} H^{(1)}_{n'''n}}{(E^0_n - E^0_{n'})(E^0_n - E^0_{n''})(E^0_n - E^0_{n'''})} + \frac{H^{(1)}_{nn'} H^{(1)}_{n'n''} H^{(1)}_{n''n'''} H^{(1)}_{n'''n}}{(E^0_n - E^0_{n'})(E^0_n - E^0_{n''})(E^0_{n''} - E^0_{n'''})} + \frac{H^{(1)}_{nn'''} H^{(1)}_{n'''n''} H^{(1)}_{n''n'} H^{(1)}_{n'n}}{(E^0_n - E^0_{n'})(E^0_n - E^0_{n''})(E^0_n - E^0_{n'''})} + \frac{H^{(1)}_{nn'''} H^{(1)}_{n'''n''} H^{(1)}_{n''n'} H^{(1)}_{n'n}}{(E^0_n - E^0_{n'})(E^0_n - E^0_{n''})(E^0_{n''} - E^0_{n'''})} \right\} .$$

The first two factors appear in the desired form, the last two do not. In order to modify them, one interchanges n''' and n', and obtains

$$\frac{5}{24} \sum_{n'\neq n} \sum_{n''\neq n, n'} \sum_{n'''\neq n, n', n''} \left\{ \frac{H^{(1)}_{nn'} H^{(1)}_{n'n''} H^{(1)}_{n''n'''} H^{(1)}_{n'''n}}{(E^0_n - E^0_{n'''})(E^0_n - E^0_{n''})(E^0_n - E^0_{n'})} + \frac{H^{(1)}_{nn'} H^{(1)}_{n'n''} H^{(1)}_{n''n'''} H^{(1)}_{n'''n}}{(E^0_n - E^0_{n'''})(E^0_n - E^0_{n''})(E^0_{n''} - E^0_{n'})} \right\}$$

Applying the same analysis to the rest of the terms, one obtains the following set of factors* (including the ones above):

$$\sum_{n' \neq n} \; \sum_{n'' \neq n', n} \; \sum_{n''' \neq n'', n', n} \left[\frac{10 \, H^{(1)}_{\cdots}}{24 \, (E^0_n - E^0_{n'})(E^0_n - E^0_{n''})(E^0_n - E^0_{n'''})} \right.$$

$$+ \frac{5}{24} \frac{H^{(1)}_{\cdots}}{(E^0_n - E^0_{n'})(E^0_n - E^0_{n''})(E^0_{n''} - E^0_{n'''})} - \frac{5}{24} \frac{H^{(1)}_{\cdots}}{(E^0_n - E^0_{n''})(E^0_n - E^0_{n'''})(E^0_{n'} - E^0_{n''})}$$

$$+ \frac{1}{6} \frac{H^{(1)}_{\cdots}}{(E^0_n - E^0_{n'''})(E^0_{n'} - E^0_{n'''})(E^0_{n''} - E^0_{n'''})} - \frac{1}{6} \frac{H^{(1)}_{\cdots}}{(E^0_n - E^0_{n'''})(E^0_{n'} - E^0_{n'''})(E^0_{n'} - E^0_{n''})}$$

$$+ \frac{1}{6} \frac{H^{(1)}_{\cdots}}{(E^0_n - E^0_{n'})(E^0_{n'} - E^0_{n'''})(E^0_{n'} - E^0_{n''})} - \frac{1}{6} \frac{H^{(1)}_{\cdots}}{(E^0_n - E^0_{n'})(E^0_{n'} - E^0_{n'''})(E^0_{n''} - E^0_{n'''})}$$

$$+ \frac{1}{24} \frac{H^{(1)}_{\cdots}}{(E^0_n - E^0_{n'})(E^0_{n'} - E^0_{n''})(E^0_n - E^0_{n'''})} + \frac{1}{24} \frac{H^{(1)}_{\cdots}}{(E^0_n - E^0_{n'})(E^0_{n'} - E^0_{n''})(E^0_{n''} - E^0_{n'''})}$$

$$- \frac{1}{24} \frac{H^{(1)}_{\cdots}}{(E^0_n - E^0_{n'''})(E^0_{n''} - E^0_{n'''})(E^0_n - E^0_{n'})} + \frac{1}{24} \frac{H^{(1)}_{\cdots}}{(E^0_n - E^0_{n'''})(E^0_{n''} - E^0_{n'''})(E^0_{n'} - E^0_{n''})}$$

$$- \frac{1}{24} \frac{H^{(1)}_{\cdots}}{(E^0_n - E^0_{n'''})(E^0_n - E^0_{n'})(E^0_{n''} - E^0_{n'''})} + \frac{1}{24} \frac{H^{(1)}_{\cdots}}{(E^0_n - E^0_{n'''})(E^0_n - E^0_{n'})(E^0_{n'} - E^0_{n''})}$$

$$+ \frac{1}{24} \frac{H^{(1)}_{\cdots}}{(E^0_n - E^0_{n'})(E_n - E^0_{n'''})(E^0_{n'} - E^0_{n''})} - \frac{1}{24} \frac{H^{(1)}_{\cdots}}{(E^0_n - E^0_{n'})(E^0_n - E^0_{n'''})(E^0_{n''} - E^0_{n'''})}$$

* This form will be denoted by $H^{(1)}\ldots$ in this part of the discussion to make things easier to write.

$$-\frac{1}{24}\frac{H^{(1)}_{\dots}}{(E^0_n-E^0_{n''})(E^0_{n'}-E^0_{n''})(E^0_n-E^0_{n'''})}-\frac{1}{24}\frac{H^{(1)}_{\dots}}{(E^0_n-E^0_{n''})(E^0_{n'}-E^0_{n''})(E^0_{n''}-E^0_{n'''})}$$

$$\left.+\frac{1}{24}\frac{H^{(1)}_{\dots}}{(E^0_n-E^0_{n''})(E^0_{n''}-E^0_{n'''})(E^0_n-E^0_{n'})}-\frac{1}{24}\frac{H^{(1)}_{\dots}}{(E^0_n-E^0_{n''})(E^0_{n''}-E^0_{n'''})(E^0_{n'}-E^0_{n''})}\right].$$

Some of the above factors required two index changes to bring them into the desired order. For example, in the last factor above, n''' and n'' were interchanged first, then n'' and n'. To combine the above factors, it will be necessary to identify each factor by "factor number" 1, 2, ... depending on the order in which they are found. With this in mind, one can recombine the above factors, as follows:

Factor numbers (4) and (7) give

$$\frac{1}{6}\frac{H^{(1)}_{\dots}}{(E^0_{n'}-E^0_{n'''})(E^0_{n''}-E^0_{n'''})}\left(\frac{1}{E^0_n-E^0_{n'''}}-\frac{1}{E^0_n-E^0_{n'}}\right)=\frac{-H^{(1)}_{\dots}}{6(E^0_{n''}-E^0_{n'''})(E^0_n-E^0_{n'''})(E^0_n-E^0_{n'})}.$$

This result then combines with factor numbers (10) and (12), giving

$$\frac{-6}{24}\frac{H^{(1)}_{\dots}}{(E^0_n-E^0_{n'})(E^0_n-E^0_{n'''})(E^0_{n''}-E^0_{n'''})}. \qquad (A')$$

Factor numbers (5) and (6) give

$$\frac{1}{6}\frac{H^{(1)}_{\dots}}{(E^0_{n'}-E^0_{n'''})(E^0_{n'}-E^0_{n''})}\left(\frac{1}{E^0_n-E^0_{n'}}-\frac{1}{E^0_n-E^0_{n'''}}\right)=\frac{H^{(1)}_{\dots}}{6(E^0_{n'}-E^0_{n''})(E^0_n-E^0_{n'})(E^0_n-E^0_{n'''})}.$$

This result, in turn, combines with factor numbers (13) and (14) to give

$$\frac{6}{24}\frac{H^{(1)}_{\dots}}{(E^0_n-E^0_{n'})(E^0_n-E^0_{n'''})(E^0_{n'}-E^0_{n''})}. \qquad (B')$$

Factor numbers (8) and (16) give

$$\frac{1}{24}\frac{H^{(1)}_{\dots}}{(E^0_{n'}-E^0_{n''})(E^0_n-E^0_{n'''})}\left(\frac{1}{E^0_n-E^0_{n'}}-\frac{1}{E^0_n-E^0_{n''}}\right)=\frac{H^{(1)}_{\dots}}{24(E^0_n-E^0_{n'''})(E^0_n-E^0_{n''})(E^0_n-E^0_{n'})}\,. \qquad (C')$$

Factor numbers (15) and (18) combine to give

$$\frac{1}{24}\frac{H^{(1)}_{\dots}}{(E^0_{n''}-E^0_{n'''})(E^0_n-E^0_{n'})}\left(\frac{1}{E^0_n-E^0_{n''}}-\frac{1}{E^0_n-E^0_{n'''}}\right)=\frac{H^{(1)}_{\dots}}{(E^0_n-E^0_{n'})(E^0_n-E^0_{n'''})(E^0_n-E^0_{n''})}\,. \qquad (D')$$

Factor numbers (11) and (19) give

$$\frac{1}{24}\frac{H^{(1)}_{\dots}}{(E^0_{n''}-E^0_{n'''})(E^0_{n'}-E^0_{n''})}\left(\frac{1}{E^0_n-E^0_{n'''}}-\frac{1}{E^0_n-E^0_{n''}}\right)=\frac{-H^{(1)}_{\dots}}{24(E^0_{n'}-E^0_{n''})(E^0_n-E^0_{n''})(E^0_n-E^0_{n'''})}$$

This result, in turn, combines with factor number (3) to give

$$-\frac{6}{24}\frac{H^{(1)}_{\dots}}{(E^0_n-E^0_{n''})(E^0_n-E^0_{n'''})(E^0_{n'}-E^0_{n''})}\,. \qquad (E')$$

This result then combines with (B') to give

$$\frac{6}{24}\frac{H^{(1)}_{\dots}}{(E^0_n-E^0_{n'})(E^0_n-E^0_{n''})(E^0_n-E^0_{n'''})}\,. \qquad (F')$$

Factor numbers (9) and (17) combine to give

$$\frac{1}{24}\frac{H^{(1)}_{\dots}}{(E^0_{n''}-E^0_{n'''})(E^0_{n'}-E^0_{n''})}\left(\frac{1}{E^0_n-E^0_{n'}}-\frac{1}{E^0_n-E^0_{n''}}\right)=\frac{1}{24}\frac{H^{(1)}_{\dots}}{(E^0_{n''}-E^0_{n'''})(E^0_n-E^0_{n'})(E^0_n-E^0_{n''})}\,.$$

This result combines with factor number (2) to give

$$\frac{6}{24}\,\frac{H^{(1)}_{\cdots}}{(E^0_{n''}-E^0_{n'''})\,(E^0_n-E^0_{n'})\,(E^0_n-E^0_{n''})}\,. \qquad (G')$$

Combining (G') with (A') one obtains

$$\frac{6}{24}\,\frac{H^{(1)}_{\cdots}}{(E^0_n-E^0_{n'})\,(E^0_n-E^0_{n''})\,(E^0_n-E^0_{n'''})}\,. \qquad (H')$$

Finally, combining factor number (1) with (C'), (D'), (F'), and (H') one obtains

$$\left(\frac{10}{24}+\frac{1}{24}+\frac{1}{24}+\frac{6}{24}+\frac{6}{24}\right)\sum_{n'\neq n}\;\sum_{n''\neq n,n'}\;\sum_{n'''\neq n,n',n''}\frac{H^{(1)}_{nn'}\,H^{(1)}_{n'n''}\,H^{(1)}_{n''n'''}\,H^{(1)}_{n'''n}}{(E^0_n-E^0_{n'})\,(E^0_n-E^0_{n''})\,(E^0_n-E^0_{n'''})}\,.$$

Note that all nineteen terms are accounted for and that the five triple sums in $E^{(4)}_n$ have now been replaced by

$$\sum_{n'\neq n}\;\sum_{n''\neq n,n'}\;\sum_{n'''\neq n,n',n''}\frac{H^{(1)}_{nn'}\,H^{(1)}_{n'n''}\,H^{(1)}_{n''n'''}\,H^{(1)}_{n'''n}}{(E^0_n-E^0_{n'})\,(E^0_n-E^0_{n''})\,(E^0_n-E^0_{n'''})}\,, \qquad (5T)$$

plus terms (ACE) and (BD).

An additional simplification in $E^{(4)}_n$ is possible by grouping the three double sums containing combinations of $H^{(1)}_{n'n}$ and $H^{(2)}_{n'n}$ matrix elements. To avoid having to rewrite the terms in question, they will be referred to as "first", "second", and "third" terms depending on the order in which they appear in $E^{(4)}_n$. Adding the first part of the first term to the first part of the second term results in

$$\frac{1}{3}\sum_{n'\neq n}\;\sum_{n''\neq n,n'}\frac{\left(H^{(1)}_{nn'}\,H^{(1)}_{n'n''}\,H^{(2)}_{n''n}+H^{(1)}_{nn''}\,H^{(1)}_{n''n'}\,H^{(2)}_{n'n}\right)}{(E^0_n-E^0_{n'})}\left(\frac{1}{E^0_n-E^0_{n''}}+\frac{1}{E^0_{n'}-E^0_{n''}}\right)\,.$$

Then, by interchanging n'' and n' in one of the factors, one gets

$$\frac{1}{3}\sum_{n'\neq n}\sum_{n''\neq n,n'}\frac{H^{(1)}_{nn'}H^{(1)}_{n'n''}H^{(2)}_{n''n}}{1}\left\{\frac{1}{E^0_n-E^0_{n'}}\left(\frac{1}{E^0_n-E^0_{n''}}+\frac{1}{E^0_{n'}-E^0_{n''}}\right)\right.$$

$$\left.+\frac{1}{E^0_n-E^0_{n''}}\left(\frac{1}{E^0_n-E^0_{n'}}-\frac{1}{E^0_{n'}-E^0_{n''}}\right)\right\}$$

$$=\frac{1}{3}\sum_{n'\neq n}\sum_{n''\neq n,n'}\frac{H^{(1)}_{nn'}H^{(1)}_{n'n''}H^{(2)}_{n''n}}{(E^0_n-E^0_{n'})(E^0_n-E^0_{n''})}\left\{\frac{(E^0_n+E^0_{n'}-2E^0_{n''})+(2E^0_{n'}-E^0_{n''}-E^0_n)}{(E^0_{n'}-E^0_{n''})}\right\}$$

$$=\sum_{n'\neq n}\sum_{n''\neq n,n'}\frac{H^{(1)}_{nn'}H^{(1)}_{n'n''}H^{(2)}_{n''n}}{(E^0_n-E^0_{n'})(E^0_n-E^0_{n''})}\;.$$

Next, add the second factor of the first term to the second factor of the second term in the same way as above. This sum is

$$\sum_{n'\neq n}\sum_{n''\neq n,n'}\frac{H^{(2)}_{nn'}H^{(1)}_{n'n''}H^{(1)}_{n''n}}{(E^0_n-E^0_{n'})(E^0_n-E^0_{n''})}\;.$$

By changing n'' to n' in the second factor of the third term, one obtains a similar expression. Combining these three terms, one obtains

$$\sum_{n'\neq n}\sum_{n''\neq n,n'}\frac{(H^{(2)}_{nn'}H^{(1)}_{n'n''}H^{(1)}_{n''n}+H^{(1)}_{nn'}H^{(2)}_{n'n''}H^{(1)}_{n''n}+H^{(1)}_{nn'}H^{(1)}_{n'n''}H^{(2)}_{n''n})}{(E^0_n-E^0_{n'})\;(E^0_n-E^0_{n''})}\;. \quad (3T)$$

The last set of terms that need to be simplified in $E^{(4)}_n$ are those containing products of the form $H^{(1)}_{nn'}\,H^{(1)}_{n'n''}\,H^{(1)}_{n''n}$. The method is the same as above: One takes the terms in the order in which they appear and interchanges n'' and n' in the second factors of each term. This gives the following expression:

$$\frac{1}{3}\sum_{n'\neq n}\;\sum_{n''\neq n,n'} H^{(1)}_{nn'}\,H^{(1)}_{n'n''}\,H^{(1)}_{n''n}\left\{\frac{2(H^{(1)}_{n'n'}-H^{(1)}_{nn})}{(E^0_n-E^0_{n'})^2(E^0_n-E^0_{n''})}+\frac{2(H^{(1)}_{n''n''}-H^{(1)}_{nn})}{(E^0_n-E^0_{n''})^2(E^0_n-E^0_{n'})}\right.$$

$$+\frac{(H^{(1)}_{n'n'}-H^{(1)}_{nn})}{(E^0_n-E^0_{n'})^2(E^0_{n'}-E^0_{n''})}-\frac{(H^{(1)}_{n''n''}-H^{(1)}_{nn})}{(E^0_n-E^0_{n''})^2(E^0_{n'}-E^0_{n''})}$$

$$\left.+\frac{(H^{(1)}_{n''n''}-H^{(1)}_{n'n'})}{(E^0_n-E^0_{n'})(E^0_{n'}-E^0_{n''})^2}-\frac{(H^{(1)}_{n''n''}-H^{(1)}_{n'n'})}{(E^0_n-E^0_{n''})(E^0_{n'}-E^0_{n''})^2}\right\}.$$

Rearranging the brace, one separates the terms as follows

$$\left\{-H^{(1)}_{nn}\left[\frac{1}{(E^0_n-E^0_n)^2}\left(\frac{2}{E^0_n-E^0_{n''}}+\frac{1}{E^0_{n'}-E^0_{n''}}\right)+\frac{1}{(E^0_n-E^0_{n''})^2}\left(\frac{2}{E_n-E_{n'}}-\frac{1}{E^0_{n'}-E^0_{n''}}\right)\right]\right.$$

$$+H^{(1)}_{n'n'}\left[\frac{1}{(E^0_n-E^0_{n'})^2}\left(\frac{2}{E^0_n-E^0_{n''}}+\frac{1}{E^0_{n'}-E^0_{n''}}\right)+\frac{1}{(E^0_{n'}-E^0_{n''})^2}\left(\frac{1}{E^0_n-E^0_{n''}}-\frac{1}{E_n-E_{n'}}\right)\right]$$

$$\left.+H^{(1)}_{n''n''}\left[\frac{1}{(E^0_n-E^0_{n''})^2}\left(\frac{2}{E^0_n-E^0_{n'}}-\frac{1}{E^0_{n'}-E^0_{n''}}\right)+\frac{1}{(E^0_{n'}-E^0_{n''})^2}\left(\frac{1}{E^0_n-E^0_{n'}}-\frac{1}{E^0_n-E^0_{n''}}\right)\right]\right\}$$

$$=\left\{\frac{-H^{(1)}_{nn}}{(E^0_n-E^0_{n''})(E^0_n-E^0_{n'})(E^0_{n'}-E_{n''})}\left(\frac{2(E^0_{n'}-E^0_{n''})+(E^0_n-E^0_{n''})}{(E^0_n-E^0_{n'})}+\frac{2(E^0_{n'}-E^0_{n''})-(E^0_n-E^0_{n'})}{(E^0_n-E^0_{n''})}\right)\right.$$

$$+\frac{H^{(1)}_{n'n'}\,[2(E^0_{n'}-E^0_{n''})+(E^0_n-E^0_{n''})-(E^0_n-E^0_{n'})]}{(E^0_n-E^0_{n'})^2\,(E^0_n-E^0_{n''})\,(E^0_{n'}-E^0_{n''})}$$

$$+ \frac{H^{(1)}_{n''n''}\left[2(E^0_{n'}-E^0_{n''}) - (E^0_n - E^0_{n'}) + (E^0_n - E^0_{n''})\right]}{(E^0_n-E^0_{n'})\,(E^0_n-E^0_{n''})^2\,(E^0_{n'}-E^0_{n''})}\Bigg\} \quad .$$

With a little extra effort on the first parenthesis, one simplifies the brace as follows:

$$\left\{\frac{3\,H^{(1)}_{n''n''}}{(E^0_n-E^0_{n'})\,(E^0_n-E^0_{n''})^2} + \frac{3\,H^{(1)}_{n'n'}}{(E^0_n-E^0_{n'})^2\,(E^0_n-E^0_{n''})} - \frac{3\,H^{(1)}_{nn}\,(2E^0_n-E^0_{n'}-E^0_{n''})}{(E^0_n-E^0_{n''})^2\,(E^0_n-E^0_{n'})^2}\right\} \quad .$$

Thus, the group of terms just considered equals

$$\sum_{n'\neq n}\ \sum_{n''\neq n,n'} \frac{H^{(1)}_{nn'}\,H^{(1)}_{n'n''}\,H^{(1)}_{n''n}}{(E^0_n-E^0_{n'})\,(E^0_n-E^0_{n''})}\left\{\frac{H^{(1)}_{n''n''}}{E^0_n-E^0_{n''}} + \frac{H^{(1)}_{n'n'}}{E^0_n-E^0_{n'}}\right\}$$

$$- H^{(1)}_{nn} \sum_{n'\neq n}\ \sum_{n''\neq n,n'} \frac{H^{(1)}_{nn'}\,H^{(1)}_{n'n''}\,H^{(1)}_{n''n}\,(2E^0_n - E^0_{n'} - E^0_{n''})}{(E^0_n - E^0_{n'})^2\,(E^0_n - E^0_{n''})^2} \qquad (4T)$$

At this point, it is best to write down $E^{(4)}_n$ incorporating all the simplifications just obtained and the additional terms generated. One obtains for $E^{(4)}_n$ the following (continued on next page):

$$
E_n^{(4)} = H_{nn}^{(4)} + \sum_{n' \neq n} \left\{ \frac{H_{nn'}^{(2)} H_{n'n}^{(2)}}{(E_n^0 - E_{n'})} + \frac{H_{nn'}^{(1)} H_{n'n}^{(3)} + H_{nn'}^{(3)} H_{n'n}^{(1)}}{(E_n^0 - E_{n'}^0)} \right.
$$

$$
+ \frac{H_{nn'}^{(1)} H_{n'n}^{(1)} (H_{n'n'}^{(1)} - H_{nn}^{(1)})^2}{(E_n^0 - E_{n'}^0)^3} + (H_{nn'}^{(1)} \frac{H_{n'n}^{(2)} + H_{nn'}^{(2)} H_{n'n}^{(1)}) (H_{n'n'}^{(1)} - H_{nn}^{(1)})}{(E_n^0 - E_{n'}^0)^2}
$$

$$
\left. + \frac{H_{nn'}^{(1)} H_{n'n}^{(1)} (E_{n'}^{(2)} - E_n^{(2)})}{2\ (E_n^0 - E_{n'}^0)^2} + \frac{H_{nn'}^{(1)} H_{n'n}^{(1)} (H_{n'n'}^{(2)} - H_{nn}^{(2)})}{2\ (E_n^0 - E_{n'}^0)^2} \right\}
$$

$$
+ \sum_{n' \neq n} \sum_{n'' \neq n, n'} \frac{H_{nn'}^{(1)} H_{n'n''}^{(1)} H_{n''n}^{(1)}}{(E_n^0 - E_{n'}^0)\ (E_n^0 - E_{n''}^0)} \left(\frac{H_{n''n''}^{(1)}}{E_n^0 - E_{n''}^0} + \frac{H_{n'n'}^{(1)}}{E_n^0 - E_{n'}^0} \right)
$$

$$
- H_{nn}^{(1)} \sum_{n' \neq n} \sum_{n'' \neq n, n'} \frac{H_{nn'}^{(1)} H_{n'n''}^{(1)} H_{n''n}^{(1)} (2E_n^0 - E_{n'}^0 - E_{n''}^0)}{(E_n^0 - E_{n'}^0)^2\ (E_n^0 - E_{n''}^0)^2}
$$

$$
+ \sum_{n' \neq n} \sum_{n'' \neq n, n'} \frac{(H_{nn'}^{(2)} H_{n'n''}^{(1)} H_{n''n}^{(1)} + H_{nn'}^{(1)} H_{n'n''}^{(2)} H_{n''n}^{(1)} + H_{nn'}^{(1)} H_{n'n''}^{(1)} H_{n''n}^{(2)})}{(E_n^0 - E_{n'}^0)\ (E_n^0 - E_{n''}^0)}
$$

$$
+ \sum_{n' \neq n} \sum_{n'' \neq n, n'} \sum_{n''' \neq n, n', n''} \frac{H_{nn'}^{(1)} H_{n'n''}^{(1)} H_{n''n'''}^{(1)} H_{n'''n}^{(1)}}{(E_n^0 - E_{n'}^0)(E_n^0 - E_{n''}^0)(E_n^0 - E_{n'''}^0)}
$$

$$
+ \frac{1}{2} \sum_{n' \neq n} \sum_{n'' \neq n, n'} \frac{H_{nn'}^{(1)} H_{n'n''}^{(1)} H_{n''n'}^{(1)} H_{n'n}^{(1)}}{(E_n^0 - E_{n'}^0)\ (E_n^0 - E_{n''}^0)} \left(\frac{1}{E_n^0 - E_{n'}^0} - \frac{1}{E_n - E_{n''}} \right)
$$

$$
- \frac{1}{4} \sum_{n' \neq n} \sum_{n'' \neq n, n'} \frac{H_{nn''}^{(1)} H_{n''n}^{(1)} H_{nn'}^{(1)} H_{n'n}^{(1)}}{(E_n^0 - E_{n'}^0)\ (E_n^0 - E_{n''}^0)} \left(\frac{1}{E_n^0 - E_{n'}^0} + \frac{1}{E_n^0 - E_{n''}^0} \right) .
$$

The last two terms correspond to terms (ACE) and (BD). These terms will combine with others generated by increasing the range on n'' and n''' later on.

Since the result for $E_n^{(4)}$ is now expressed in terms of denominators which exclude factors of the form $(E^0_{n'}-E^0_{n''})$, $(E^0_{n'}-E^0_{n'''})$, and $(E^0_{n''}-E^0_{n'''})$, one may now put back those terms which are not affected by this type of singularity. The last two terms do not fit this description, but as was pointed out earlier, they will combine properly when all the modifications are included.

One may now express $E_n^{(4)}$ in terms of sums having the following form:*

$$\sum_{n'\neq n} Q \ , \qquad \sum_{n'\neq n}\ \sum_{n''\neq n} Q \ , \qquad \sum_{n'\neq n}\ \sum_{n''\neq n}\ \sum_{n'''\neq n} Q \ .$$

Thus to change the double sums one needs to take

$$\sum_{n'\neq n}\ \sum_{n''\neq n,n'} Q = \sum_{n'\neq n}\ \sum_{n''\neq n} Q - \sum_{n'\neq n} Q\ (n''=n').$$

With this in mind, one replaces the triple sum term in $E_n^{(4)}$ by

$$\sum_{n'\neq n}\ \sum_{n''\neq n}\ \sum_{n'''\neq n} \frac{H^{(1)}_{nn'}\,H^{(1)}_{n'n''}\,H^{(1)}_{n''n'''}\,H^{(1)}_{n'''n}}{(E^0_n-E^0_{n'})(E^0_n-E^0_{n''})(E^0_n-E^0_{n'''})}$$

$$-\sum_{n'\neq n}\ \sum_{n''\neq n,n'} \frac{(H^{(1)}_{nn'}\,H^{(1)}_{n'n''}\,H^{(1)}_{n''n'}\,H^{(1)}_{n'n})}{(E^0_n-E^0_{n'})^2\,(E^0_n-E^0_{n''})}$$

$$-\sum_{n'\neq n}\ \sum_{n''\neq n,n'} \frac{H^{(1)}_{nn'}\,H^{(1)}_{n'n''}\,H^{(1)}_{n''n}}{(E^0_n-E^0_{n'})\,(E^0_n-E^0_{n''})}\left(\frac{H^{(1)}_{n''n''}}{E^0_n-E^0_{n''}}+\frac{H^{(1)}_{n'n'}}{E^0_n-E^0_{n'}}\right) \qquad \text{(v)}$$

* Let Q denote any given expression.

The newly generated double sums are incorporated into the existing terms in $E_n^{(4)}$ before the above modification of the double sums is performed. In doing this one notes that the last term in (v) cancels one of the terms in $E_n^{(4)}$, the second term in (v) adds to the next to the last term in $E_n^{(4)}$. This last term will be incorporated later on. In referring to $E_n^{(4)}$, one notes that the next term to be simplified is the second double sum. When this term is modified, one obtains

$$- H_{nn}^{(1)} \sum_{n'\neq n} \sum_{n''\neq n} \frac{H_{nn'}^{(1)} H_{n'n''}^{(1)} H_{n''n}^{(1)} (2E_n^0 - E_{n'}^0 - E_{n''}^0)}{(E_n^0 - E_{n'}^0)^2 (E_n^0 - E_{n''}^0)^2}$$

$$+ 2 H_{nn}^{(1)} \sum_{n'\neq n} \frac{(H_{nn'}^{(1)} H_{n'n}^{(1)}) H_{n'n'}^{(1)}}{(E_n^0 - E_{n'}^0)^3} . \qquad \text{(w)}$$

The new factor generated above cancels the middle factor obtained when the fourth term in $E_n^{(4)}$ is multiplied out.* The fourth term (a double sum) of $E_n^{(4)}$ that requires modification becomes

$$\sum_{n'\neq n} \sum_{n''\neq n} \frac{(H_{nn'}^{(2)} H_{n'n''}^{(1)} H_{n''n}^{(1)} + H_{nn'}^{(1)} H_{n'n''}^{(2)} H_{n''n}^{(1)} + H_{nn'}^{(1)} H_{n'n''}^{(1)} H_{n''n}^{(2)})}{(E_n^0 - E_{n'}^0)(E_n^0 - E_{n''}^0)}$$

$$- \sum_{n'\neq n} \frac{(H_{nn'}^{(1)} H_{n'n}^{(2)} + H_{nn'}^{(2)} H_{n'n}^{(1)}) H_{n'n'}^{(1)}}{(E_n^0 - E_{n'}^0)^2} - \sum_{n'\neq n} \frac{(H_{nn'}^{(1)} H_{n'n}^{(1)}) H_{n'n'}^{(2)}}{(E_n^0 - E_{n'}^0)^2} \qquad \text{(x)}$$

Here again, one notes that the new terms generated above cancel some of the existing terms in $E_n^{(4)}$.

Before incorporating all the terms generated one should take care of the last two terms in $E_n^{(4)}$. Combining the first term with the middle factor of (v), one obtains

---

* The last form of $E_n^{(4)}$ is referred to in each of the cases that follow.

$$-\frac{1}{2}\sum_{n'\neq n}\sum_{n''\neq n,n'}\frac{H^{(1)}_{nn'}H^{(1)}_{n'n''}H^{(1)}_{n''n'}H^{(1)}_{n'n}}{(E^0_n - E^0_{n'})^2(E^0_{n'} - E^0_{n''})}\ .$$

Now, if one puts the factor corresponding to n'' = n, back into the above expression, one obtains

$$-\frac{1}{2}\sum_{n'\neq n}\sum_{n''\neq n'}\frac{H^{(1)}_{nn'}H^{(1)}_{n'n''}H^{(1)}_{n''n'}H^{(1)}_{n'n}}{(E^0_n-E^0_{n'})^2(E^0_{n'}-E^0_{n''})} - \frac{1}{2}\sum_{n'\neq n}\frac{(H^{(1)}_{nn'}H^{(1)}_{n'n})^2}{(E^0_n-E^0_{n'})^3}\ , \quad (y)$$

(both signs are negative because, when n'' = n, $(E^0_{n'} - E^0_{n''})$ is negative). When the first term in (y) is rearranged, the result is

$$-\frac{1}{2}\sum_{n'\neq n}\frac{H^{(1)}_{nn'}}{(E^0_n-E^0_{n'})}\left(\sum_{n''\neq n'}\frac{H^{(1)}_{n'n''}H^{(1)}_{n''n'}}{(E^0_{n'}- E^0_{n''})}\right)\frac{H^{(1)}_{nn'}}{(E^0_n-E^0_{n'})}\ .$$

Now, by using equation (26) in the form

$$(E^{(2)}_{n'} - H^{(2)}_{n'n'}) = \sum_{n''\neq n'}\frac{(H^{(1)}_{n'n''}H^{(1)}_{n''n'})}{(E^0_{n'} - E^0_{n''})}\ ,$$

(y) becomes

$$-\frac{1}{2}\sum_{n'\neq n}\frac{H^{(1)}_{nn'}H^{(1)}_{n'n}(E^{(2)}_{n'} - E^{(2)}_{n})}{(E^0_n - E^0_{n'})^2} - \frac{1}{2}\sum_{n'\neq n}\frac{(H^{(1)}_{nn'}H^{(1)}_{n'n})^2}{(E^0_n-E^0_{n'})^3}\ . \quad (y')$$

By performing the above manipulations, one eliminates what appeared to be a "bad" term. The same analysis takes care of the last term in $E^{(4)}_n$. Taking out the factor corresponding to n'' = n', one obtains, for this last factor, the expression

$$-\frac{1}{4}\sum_{n'\neq n}\sum_{n''\neq n}\frac{H^{(1)}_{nn''}H^{(1)}_{n''n}H^{(1)}_{nn'}H^{(1)}_{n'n}}{(E^0_n-E^0_{n'})(E^0_n-E^0_{n''})}\left(\frac{1}{E^0_n-E^0_{n'}}+\frac{1}{E^0_n-E^0_{n''}}\right)$$

$$+\frac{1}{2}\sum_{n'\neq n}\frac{(H^{(1)}_{nn'}H^{(1)}_{n'n})^2}{(E^0_n-E^0_{n'})^3}\ . \qquad (z)$$

Now, by separating out terms in the first factor above and by using equation (26), one obtains

$$-\frac{1}{4}\sum_{n'\neq n}\frac{(E^{(2)}_n-H^{(2)}_{nn})H^{(1)}_{nn'}H^{(1)}_{n'n}}{(E^0_n-E^0_{n'})^2}-\frac{1}{4}\sum_{n''\neq n}\frac{H^{(1)}_{nn''}H^{(1)}_{n''n}(E^{(2)}_n-H^{(2)}_{nn})}{(E^0_n-E^0_{n''})^2}.$$

Let n'' = n' in the second term above, and equation (z) becomes

$$-\frac{1}{2}\sum_{n'\neq n}\frac{H^{(1)}_{nn'}H^{(1)}_{n'n}(E^{(2)}_n-H^{(2)}_{nn})}{(E^0_n-E^0_{n'})^2}+\sum_{n'\neq n}\frac{(H^{(1)}_{nn'}H^{(1)}_{n'n})^2}{2(E^0_n-E^0_{n'})^3} \qquad (z')$$

By combining (y') and (z') and all the other terms generated, one finally obtains (continued on next page):

$$E_n^{(4)} = H_{nn}^{(4)} + \sum_{n' \neq n} \frac{\left(H_{nn'}^{(1)} H_{n'n}^{(3)} + H_{nn'}^{(3)} H_{n'n}^{(1)}\right)}{\left(E_n^0 - E_{n'}^0\right)} + \sum_{n' \neq n} \frac{H_{nn'}^{(2)} H_{n'n}^{(2)}}{\left(E_n^0 - E_{n'}^0\right)}$$

$$- E_n^{(2)} \sum_{n' \neq n} \frac{H_{nn'}^{(1)} H_{n'n}^{(1)}}{\left(E_n^0 - E_{n'}^0\right)^2} + \sum_{n' \neq n} \frac{H_{nn'}^{(1)} H_{n'n}^{(1)} \left[\left(H_{n'n'}^{(1)}\right)^2 + \left(H_{nn}^{(1)}\right)^2\right]}{\left(E_n^0 - E_{n'}^0\right)^3}$$

$$- H_{nn}^{(1)} \sum_{n' \neq n} \sum_{n'' \neq n} \frac{\left(H_{nn'}^{(1)} H_{n'n''}^{(1)} H_{n''n}^{(1)}\right) \left(2E_n^0 - E_{n'}^0 - E_{n''}^0\right)}{\left(E_n^0 - E_{n'}^0\right)^2 \left(E_n^0 - E_{n''}^0\right)^2}$$

$$+ \sum_{n' \neq n} \sum_{n'' \neq n} \frac{\left(H_{nn'}^{(2)} H_{n'n''}^{(1)} H_{n''n}^{(1)} + H_{nn'}^{(1)} H_{n'n''}^{(2)} H_{n''n}^{(1)} + H_{nn'}^{(1)} H_{n'n''}^{(1)} H_{n''n}^{(2)}\right)}{\left(E_n^0 - E_{n'}^0\right) \left(E_n^0 - E_{n''}^0\right)}$$

$$+ \sum_{n' \neq n} \sum_{n'' \neq n} \sum_{n''' \neq n} \frac{\left(H_{nn'}^{(1)} H_{n'n''}^{(1)} H_{n''n'''}^{(1)} H_{n'''n}^{(1)}\right)}{\left(E_n^0 - E_{n'}^0\right)\left(E_n^0 - E_{n''}^0\right)\left(E_n^0 - E_{n'''}^0\right)} .$$

This answer may now be used for numerical calculations requiring perturbation terms up to fourth order. With the aid of computers this type of calculation is becoming more prevalent.

George C. Marshall Space Flight Center
National Aeronautics and Space Administration
November 1965

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