ALGEBRAIC FORMULATION OF THE OPERATORIAL PERTURBATION THEORY. PART I

Ary W. Espinosa Müller
Departamento de Física, Universidad de Concepción
Casilla 4009, Concepción, Chile

Adelio R. Matamala Vásquez
Departamento de Físico–Química, Universidad de Concepción
Casilla 3–C, Concepción, Chile

April 1, 2022

Abstract

A new totally algebraic formalism based on general, abstract ladder operators has been proposed. This approach heavily grounds in the superoperator formalism of Primas. However it is necessary to introduce many improvements in his formalism. In this regard, it has been introduced a new set of superoperators featured by their algebraic structure. Also, two lemmas and one theorem have been developed in order to algebraically reformulate the theory on more rigorous grounds. Finally, we have been able to build a coherent and self-contained formalism independent on any matricial representation, removing in this way the degeneracy problem.
1 INTRODUCTION

The fundamental problem in perturbation theory is the solution of the Schrödinger equation

$$\hat{H}\Psi = E\Psi,$$  \hspace{1cm} (1)

for the stationary states $\Psi(x, y, z)$ of a system where the Hamiltonian $\hat{H}$ is split into an unperturbed Hamiltonian $\hat{H}^o$ and a perturbation $\hat{V}$. Traditional treatments of the theory lean heavily on the expansion of correction to an eigenfunction in terms of a complete set of normalized eigenfunctions of $\hat{H}^o$ [1–4]. However, the problem can also be formulated in terms of obtaining an effective Hamiltonian $\hat{M} = \hat{U}\hat{H}\hat{U}^\dagger$, with $\hat{U}$ a unitary operator. The unitary or canonical transformation [5] method originated by Van Vleck [6], has been adopted by Prima [7], Jørgensen and Pedersen [8], Mukherjee et al. [9] and others [10]. The $\hat{U}$ operator is unitary in the Van Vleck and Prima’s formalism and produces a Hermitian effective Hamiltonian.

Murray [11] and Prima [7], have been able to show that any perturbation theory can be formulated in the domain of the Lie algebras, in this case generated by $\hat{H}^o$ and $\hat{V}$. In that concern, the solution of a perturbation problem is closely connected with the solution of commutator equations of a given type. Further, using the spectral resolution of $\hat{H}^o$, Prima was able to show that the general solution can be written more adequately with the aid of the superoperator algebra.

In the above scenario, our main aim is to recast the superoperator formalism of Prima in an algebraic form using, to that end, the basic theory of ladder operators [12] thus our work will be reduced to prove that formally it is always possible to build a realization. In Part 2 of this series, we will show how particular realizations will lead us to successfully check the present approach to of the perturbation theory (AFOPT, Algebraic Formulation of the Operator Perturbation Theory).

The above AFOPT avoids the matrix representation, since as it is well known in the commonly used treatments, the perturbative series and hence the expectation values of $\hat{H}$, depend crucially on the orthonormal eigenbase of $\hat{H}^o$.

The outline of the paper is as follow. The treatment begins with the definition of the eigenbase $\{|n^o\rangle\}$ of $\hat{H}^o$. Then, the ladder operators defined
in this eigenbase have been presented with their main characteristics. At the same time in this Sect. 2 the multilinear operators $\hat{\eta}_m^m \hat{\eta}_n^n$ and $\hat{\eta}_m^m \hat{\eta}_n^n$ have been stated. These operators will serve to establish a resolution of any operator belonging to the operator space $\mathcal{T}$, whose base has been given by $\{|n^o\rangle\}$. In Sect. 3, two lemmas and one fundamental theorem to of the AFOPT are presented. In Sect. 4, the perturbation operator theory is briefly presented. This section is followed by a summary and discussions in Sect. 5 Finally, the paper ends up with the mnemonic technique in order to write the commutator equations.

2 FORMALISM

2.1 LADDER OPERATORS

The full Hamiltonian $\hat{H}$ is split into a zero-order Hamiltonian $\hat{H}^o$ and a perturbation $\hat{V}$

$$\hat{H} = \hat{H}^o + \lambda \hat{V}, \text{with } \lambda \in [0, 1]$$

Orthonormal eigenkets of $\hat{H}^o$ which belong to the zeroth-order eigenspace of energy $\varepsilon^o_n$ are denoted by $|n^o\rangle$

$$\hat{H}|n^o\rangle = \varepsilon^o_n|n^o\rangle$$

As the perturbation is switched on the zero-order eigenkets $|n^o\rangle$ evolves into orthonormal perturbed eigenkets $|n\rangle$ of energy $\varepsilon_n$.

Some time ago, De la Peña and Montemayor [12–16] have shown that given the discrete spectral resolution of a linear and Hermitian operator $\hat{P}$, it is always possible to construct raising and lowering operators associated to that operator. Hence, related to $\hat{H}^o$ we have at our disposal the discrete eigenbase $\{|n^o\rangle\}$, thus we may state with all generality

$$\hat{\eta}_+ = \sum_n c_n|n + 1\rangle\langle n|$$

and

$$\hat{\eta}_- = \sum_n c^*_n|n - 1\rangle\langle n|$$
From the orthonormality condition it is easy to see that \( \hat{\eta}_+ \) and \( \hat{\eta}_- \) are ladder operators

\[
\hat{\eta}_+ |k\rangle = c_k |k + 1\rangle
\]

\[
\hat{\eta}_- |k\rangle = c_{k-1}^* |k - 1\rangle
\]

Now, since \( \hat{\eta}_+ \) and \( \hat{\eta}_- \) are adjoint to each other, the eigenbase \( \{ |n\rangle \} \) is a common eigenbase to both operators \( \hat{\eta}_+ \hat{\eta}_- \) and \( \hat{\eta}_- \hat{\eta}_+ \)

\[
\hat{\eta}_+ \hat{\eta}_- |n\rangle = |c_n|^2 |n\rangle
\]

\[
\hat{\eta}_- \hat{\eta}_+ |n\rangle = |c_{n-1}|^2 |n\rangle
\]

The coefficients \( c_n \) and \( c_{n-1}^* \) are complex number related to the eigenvalues of \( \hat{\eta}_+ \hat{\eta}_- \) and \( \hat{\eta}_- \hat{\eta}_+ \).

Furthermore, we assume that the eigenvalue spectrum is bounded from below and from above [13,17,18]

\[
\varepsilon_0^\circ < \varepsilon_1^\circ < \cdots < \varepsilon_N^\circ
\]

Therefore

\[
c_{-1} = c_M = 0
\]

From Eqs. 2.7 and 2.8 it follows that \( \hat{\eta}_+ \hat{\eta}_- \) differs from \( \hat{\eta}_- \hat{\eta}_+ \). In order to have only one kind of expressions, we adopt the normal ordering, by which the normal product of a set of raising and lowering operators is defined to be the product arranged, so that the raising operators are to the left of the lowering operators.

### 2.2 Superoperators

Now, in order to build the algebraic formulation to of the perturbation theory, let us introduce the notion of superoperator [7,18,19]. The superoperator algebra of all linear operators acting on the wavefunction space \( \mathcal{H} \), is a linear vector space, called operator space \( \mathcal{T} \). Just as we define mappings \( \hat{T} : \mathcal{H} \to \mathcal{H} \) called operators, so we can define mappings \( \tau : \mathcal{T} \to \mathcal{T} \) called
superoperators. Both kinds of mappings are linear mappings. Also, linearity, the sum and the product by scalar, of superoperators are defined analogously to the definitions for the operators. Then it is clear that the superoperator space is again a linear space. The foregoing clarification is relevant for forthcoming developments of the theory. Actually, let us look for the connection between operators and superoperators in the present algebraic approach to the perturbation theory.

So as to do that, let us consider an operator $\hat{A}$ of the operator space $\mathcal{T}$, we will assume that it is possible to write in normal ordering the following expansion

$$\hat{A} = \sum_m \sum_n a_{mn} \hat{\eta}_+^m \hat{\eta}_-^n$$

Where now the $a_{mn}$ coefficients will depend on the explicit form of the operator $\hat{A}$. It is immediate to write:

$$\hat{A} = \sum_m a_{mm} \hat{\eta}_+^m + \sum_m a_{mn} \hat{\eta}_+^m \hat{\eta}_-^n$$

Then it is possible to show that

$$[\hat{H}_0, \hat{\eta}_+^m \hat{\eta}_-^n] = \hat{0}$$

if $m = n$, and

$$[\hat{H}_0, \hat{\eta}_+^m \hat{\eta}_-^n] \neq \hat{0}$$

if $m \neq n$.

In fact, having in mind Eq. 2.2 and the expansion of the operator $\hat{A}$, we get for any ket $|k\rangle$:

$$[\hat{H}_0, \hat{\eta}_+^m \hat{\eta}_-^n] |k\rangle = (\varepsilon_{k+m-n} - \varepsilon_{k}^0) \hat{\eta}_+^m \hat{\eta}_-^n |k\rangle$$

from which the results Eq. 2.11 and Eq. 2.12 follow.

Then it is feasible to define the following operators

$$\hat{A} = \sum_m a_{mm} \hat{\eta}_+^m \hat{\eta}_-^n$$

and
\[ \hat{A}_\perp = \sum_{m \neq n} \sum a_{mn} \hat{n}_+^m \hat{n}_-^n \]  

(16)

Therefore

\[ \hat{A} = \hat{A}_\parallel + \hat{A}_\perp \]  

(17)

The operators \( \hat{A}_\parallel \) and \( \hat{A}_\perp \) are referred to as the parallel and orthogonal components of the operator \( \hat{A} \) relative to \( \hat{H}^\circ \). They satisfy the next relations:

\[ [\hat{H}^\circ, \hat{A}_\parallel] = 0 \]  

(18)

and

\[ [\hat{H}^\circ, \hat{A}_\perp] \neq 0 \]  

(19)

Since \( \hat{A} \) is any operator belonging to space \( \mathcal{T} \), we have split the operator space \( \mathcal{T} \) into two subspaces \( \mathcal{T}_\parallel \) and \( \mathcal{T}_\perp \). Where \( \mathcal{T}_\parallel \) contains all the operators that commute with \( \hat{H}^\circ \), and \( \mathcal{T}_\perp \) all the operators that do not commute with \( \hat{H}^\circ \). It is necessary to remark that

\[ \mathcal{T}_\parallel \cup \mathcal{T}_\perp = \mathcal{T} \]  

(20)

and

\[ \mathcal{T}_\parallel \cap \mathcal{T}_\perp = \{0\} \]  

(21)

As it has been pointed out, the operator space \( \mathcal{T} \) is a vector space, therefore Eq. 2.16 may be interpreted as the resolution of operator \( \hat{A} \) into two components: one parallel component relative to \( \hat{H}^\circ \) and other orthogonal component relative to \( \hat{H}^\circ \). The above remark contains the key which will lead us to prove the theorem about the existence and uniqueness of the inverse of a superoperator \( \Gamma \) (see Sect. 3). The partitioning that has been performed is equivalent to the partitioning in block-diagonal and off-diagonal of Primas [7], and this in turn is the same partitioning as the even and odd one of Jørgensen and Pedersen [8].
3 TWO LEMMAS AND ONE THEOREM

As was distinguished by Murray [20] and by Primas [7], the solution of a perturbation problem may be formulated in terms of the solution of the commutator equation of the type

\[ [\hat{H}^o, \hat{X}] = \hat{Y} \]  
(22)

where \( \hat{H}^o \) is the unperturbed Hamiltonian, \( \hat{Y} \) an operator or function of operators and \( \hat{X} \) is an unknown operator that has to be determined. Using the spectral resolution of \( \hat{H}^o \), Primas [7] has been able to state the general solution for Eq. 3.1 in the language of superoperator, as given by

\[ \hat{X} - \Pi(\hat{X}) = \Gamma^{-1}(\hat{Y}) \]  
(23)

In Eq. 3.2 \( \Pi \) represents the superoperator that projects from any operator, that part which commutes with \( \hat{H}^o \), and \( \Gamma^{-1} \) denotes the inverse of the superoperator \( \Gamma \) called derivation superoperator generated by \( \hat{H}^o \) [7]. Our task will be to reformulate Eq. 3.2 in the abstract ladder operator language. If we are able to represent the \( \Pi, \Gamma \) and \( \Gamma^{-1} \) superoperators in terms of the abstract \( \hat{\eta}^+ \) and \( \hat{\eta}^- \) ladder operators of the Sect. 2, we will have achieved the main goal of the present work. To do that, we would like to state two lemmas. Before doing that, we will define \( \Pi(\hat{X}) \) as the parallel projection of the \( \hat{X} \) operator.

**Definition:** For any linear and Hermitian operator \( \hat{X} \in \mathcal{T} \) the parallel projection will be defined by

\[ \Pi(\hat{X}) = \sum_n \langle n^o | \hat{X} | n^o \rangle | n^o \rangle | n^o \rangle \]  
(24)

**Lemma 1:** Given the abstract ladder operators \( \hat{\eta}_+ \) and \( \hat{\eta}_- \) the parallel projection superoperator defined over the multilinear operators \( \hat{\eta}_+^m \hat{\eta}_-^n \), \( m, n = 0, 1, 2, \cdots \) satisfies the following relation

\[ \Pi(\hat{\eta}_+^m \hat{\eta}_-^n) = \delta_{mn} \hat{\eta}_+^m \hat{\eta}_-^n \]  
(25)

**Proof:** The action of the multilinear operator \( \hat{\eta}_+^m \hat{\eta}_-^n \) on any ket \( |k\rangle \) may be represented by

\[ \Pi(\hat{X}), \Gamma(\hat{X}) \text{ and } \Gamma^{-1}(\hat{X}) \] in our notation correspond to \( \langle \hat{X} \rangle, k(\hat{X}) \text{ and } \frac{1}{k}(\hat{X}) \) in that of Primas [7].
\[ \hat{n}_m^m \hat{n}_n^m |k\rangle = \lambda(k; m, n) |k + m - n\rangle \]

where \( \lambda(k; m, n) \) is a multiplicative factor depending on the powers \( m \) and \( n \) and the quantum number \( k \). By definition

\[ \Pi(\hat{\eta}_m^m \hat{\eta}_n^m) = \sum_k \langle k | \hat{\eta}_m^m \hat{\eta}_n^m | k\rangle \langle k | \]

and rearranging

\[ \Pi(\hat{\eta}_m^m \hat{\eta}_n^m) = \sum_k \lambda(k; m, n) \langle k | k + m - n \rangle \langle k | \]

\[ \Pi(\hat{\eta}_m^m \hat{\eta}_n^m) = \sum_k \lambda(k; m, n) \delta_{mn} \langle k | \langle k | \]

\[ \Pi(\hat{\eta}_m^m \hat{\eta}_n^m) = \delta_{mn} \sum_k \lambda(k; m, n) \langle k | \langle k | \]

\[ \Pi(\hat{\eta}_m^m \hat{\eta}_n^m) = \delta_{mn} \hat{\eta}_m^m \hat{\eta}_n^m \]

which proves Lemma 1.

The next property derives from the definition of \( \Pi \) itself:

\[ \Pi(\alpha \hat{A} + \beta \hat{B}) = \alpha \Pi(\hat{A}) + \beta \Pi(\hat{B}) \quad (26) \]

From Eq. 3.5 and Lemma 1 it is easy to obtain the properties

\[ \Pi(\hat{A}) = \hat{A}_\parallel \quad (27) \]

\[ \Pi(\hat{A}_\parallel) = \hat{A}_\parallel \quad (28) \]

\[ \Pi(\hat{A}_\perp) = 0 \quad (29) \]

Furthermore, from Eqs.2.16 and 3.4 we may deduce the useful identity
\[ \hat{A}_\perp = \hat{A} - \Pi(\hat{A}) \]  

**Definition:** The *derivation superoperator* $\Gamma$ is given by

\[ \Gamma(\hat{X}) = [\hat{H}^\circ, \hat{X}] \]  

with $\hat{X} \in T$.

To study this superoperator, it is necessary to state the following lemma.

**Lemma 2:** Given the operator $\hat{H}^\circ$ and its ladder operators $\hat{\eta}_+$ and $\hat{\eta}_-$ the derivation superoperator of the multilinear operator $\hat{\eta}_+^m \hat{\eta}_-^n \in T$ satisfies the following general form:

\[ \Gamma(\hat{\eta}_+^m \hat{\eta}_-^n) = \hat{\eta}_+^m \hat{\eta}_-^n \sum_k (\varepsilon_k + m - n - \varepsilon_k^o) |k\rangle \langle k| \]  

**Proof:** By definition of $\Gamma$ we get

\[ \Gamma(\hat{\eta}_+^m \hat{\eta}_-^n) |k\rangle = \varepsilon_k^o \hat{\eta}_+^m \hat{\eta}_-^n |k\rangle - \varepsilon_k \hat{\eta}_+^m \hat{\eta}_-^n |k\rangle \]

Multiplying to the right by the bra $\langle k|$ and summing up, it follows

\[ \Gamma(\hat{\eta}_+^m \hat{\eta}_-^n) = \sum_k (\varepsilon_k^o + m - n - \varepsilon_k^o) \hat{\eta}_+^m \hat{\eta}_-^n |k\rangle \langle k| \]

From which Lemma 2 has been proved.

The next properties are easily derived from the definition of the $\Gamma$ superoperator.

Since $\Gamma$ is a linear superoperator one has

\[ \Gamma(\alpha A + \beta B) = \alpha \Gamma(A) + \beta \Gamma(B) \]  

Also, it is immediate that

\[ \Gamma(\hat{A}_\parallel) = 0 \]  

and since $\Gamma$ is the superoperator which forms the commutator from any operator of $T$ with $\hat{H}^\circ$, one gets
\[ \Gamma(\hat{A}\hat{B}) = \hat{A}\Gamma(\hat{B}) + \Gamma(\hat{A})\hat{B} \] (37)

The superoperator \( \Gamma \) obtains its name from its derivative properties.

Some comments must be deserved to the last two lemmas. Firstly, from Eq. 3.4 one realizes that the action of \( \Pi \) is independent on the physics of the system, since the Hamiltonian has not been considered explicitly. Hence the superoperator \( \Pi \) simply split the entire operator space into two subspaces (orthogonal and parallel). Secondly, Eq. 3.6 points out directly, that the action of \( \Gamma \) has an explicit dependence on \( \hat{H}^o \), due to the presence of the transition energy \( \Delta \varepsilon^o = \varepsilon^o_{k+m-n} - \varepsilon^o_k \), which is also an immediate consequence of the definition of \( \Gamma \) itself.

One very fundamental question to build a coherent and self contained algebraic perturbation theory, is to assure the existence of the superoperator \( \Gamma^{-1} \) in the Primas’ theory. Primas has prevented from demonstrating this relevant theorem because he considers that the inverse superoperator \( \Gamma^{-1} \) has the whole operator space \( \mathcal{T} \) as its domain \([7]\). On the contrary, we will show that \( \Gamma^{-1} \) exists solely in the orthogonal subspace \( \mathcal{T}_\perp \subset \mathcal{T} \). Therefore, we aim to discover the proper arguments leading to demonstrate the existence and uniqueness of inverse superoperator. A subject that we will now study in somewhat greater detail.

**THEOREM:** The inverse superoperator \( \Gamma^{-1} \) exists and it is unique, if and only if the domain and the range of the linear mapping associated with it, can be adequately restricted to the orthogonal subspace \( \mathcal{T}_\perp \subset \mathcal{T} \).

**Proof:** Since the superoperator \( \Gamma \) is a linear mapping, it allows us to introduce the kernel of a linear mapping \([21]\) and hence the kernel of the superoperator \( \Gamma \), which we denote by \( \text{ker} \Gamma \), and that we define as the set of all the operators \( \hat{X} \in \mathcal{T} \) such that \( \Gamma(\hat{X}) = \hat{0} \).

Having in mind that a linear mapping whose kernel is \( \{\hat{0}\} \), is injective \([21,22]\), we find that \( \Gamma \), defined by

\[ \Gamma : \mathcal{T} \to \mathcal{T} \] (38)

with

\[ \Gamma(\hat{X}) = [\hat{H}^o, \hat{X}] \]

is not an injective mapping. Really, Eqs 3.14 and 3.15 show that \( \text{ker} \Gamma = \mathcal{T}_\parallel \neq \{\hat{0}\} \). However, it is possible to redefine the domain and the range of the
mapping $\Gamma$ to the orthogonal subspace, since $\Pi(\Gamma(\hat{X})) = \hat{0}$. Thus redefining
the mapping $\Gamma$ by :

$$\Gamma : \mathcal{T}_\perp \to \mathcal{T}_\perp$$

(39)

with

$$\Gamma(\hat{X}) = [\hat{H}^\circ, \hat{X}]$$

we succeed in getting $\ker \Gamma = \{\hat{0}\}$.

Actually, if we assume that an arbitrary orthogonal operator, $\hat{A} \in \mathcal{T}_\perp$, is
such that $\hat{A} \in \ker \Gamma$, then $\Gamma(\hat{A}) = \hat{0}$. But, we know that $\Gamma(\hat{A}) \neq \hat{0}$ if $\hat{A} \in \mathcal{T}_\perp$, then the assumption is false. Hence the unique element of the $\ker \Gamma$ is $\hat{0}$. In
other words, $\Gamma$ is injective. Otherwise, the image and the range of $\Gamma$ are the
same, so $\Gamma$ must be surjective. Therefore, the inverse of the $\Gamma$ exists and is
unique. Hence, by fair means we can now write

$$\Gamma^{-1}(\Gamma(\hat{X})) = \Gamma(\Gamma^{-1}(\hat{X})) = \hat{X}$$

(40)

if and only if

$$\hat{X} \in \mathcal{T}_\perp$$

(41)

and the Theorem has been proved.

Lastly the following properties are evident from $\Gamma^{-1}$, since the linearity of
$\Gamma^{-1}$ follows from the linearity of $\Gamma$,

$$\Gamma^{-1}(\alpha \hat{A} + \beta \hat{B}) = \alpha \Gamma^{-1}(\hat{A}) + \beta \Gamma^{-1}(\hat{B})$$

(42)

Thus the perturbational problem has been reduced to the finding of an explicit expression for $\Gamma^{-1}$. In Part 2 of this series, we will study particular forms for $\Gamma^{-1}$ (also for $\Gamma$ and $\Pi$), depending on the algebra of ladder operators associated to the physical problem to be tackled.

4 PERTURBATION METHOD

As aforementioned the complete Hamiltonian $\hat{H}$ has been split into an un-
perturbed Hamiltonian $H^\circ$ and a perturbation operator $V$ scaling with the
real parameter $\lambda \in [0, 1]$. 

11
\[ \hat{H} = \hat{H}^\circ + \lambda \hat{V} \quad (43) \]

Besides, the comments that have been made at the beginning of Sect. 2 (cf. Eqs. 2.1 and 2.2) also special mention deserves the fact that in general

\[ [\hat{H}^\circ, \hat{V}] \neq 0 \quad (44) \]

which implies that we cannot find a common eigenbase for \( \hat{H}^\circ \) and \( \hat{V} \). But we can think of a certain unitary transformation, that will change this situation.

The idea of choosing a unitary transformation corresponds to the need of leaving invariant the spectrum of eigenvalues of the energy. The unitary transformation only modifies the eigenvectors.

Let \( \hat{U} \) be a unitary transformation defined as

\[ \hat{U} \hat{H} \hat{U}^\dagger = \hat{U}(\hat{H}^\circ + \lambda \hat{V}) \hat{U}^\dagger \quad (45) \]

We can now introduce two new operators \( \hat{M} \) and \( \hat{W} \), through the definitions

\[ \hat{M} = \hat{U} \hat{H} \hat{U}^\dagger \quad (46) \]

and

\[ \hat{W} = \hat{M} - \hat{H}^\circ \quad (47) \]

The relation 4.4 allows to write

\[ \hat{M} = \hat{H}^\circ + \hat{W} \quad (48) \]

From Eq. 4.4 it is immediate to see that \( \hat{M} \) has the same spectrum of eigenvalues as the Hamiltonian \( \hat{H} \).

We will now suppose that \( \hat{U} \) satisfies the following condition

\[ [\hat{H}^\circ, \hat{W}] = 0 \quad (49) \]

That means that \( \hat{H}^\circ \) and \( \hat{M} \) will have common eigenvectors as follows from Eq. 4.6. Therefore, if Eq. 4.7 holds, we may write

\[ \langle n^\circ | \hat{M} | n^\circ \rangle = \langle n^\circ | \hat{H}^\circ | n^\circ \rangle + \langle n^\circ | \hat{W} | n^\circ \rangle \quad (50) \]
\[ \varepsilon_n = \varepsilon_n^o + \langle n^o | \hat{W} | n^o \rangle \]  

(51)

Since \( \langle n^o | \hat{M} | n^o \rangle = \varepsilon_n \) and \( \hat{M} = \hat{U} \hat{H} \hat{U}^\dagger \) we may write

\[ \hat{U} \hat{H} \hat{U}^\dagger | n^o \rangle = \varepsilon_n | n^o \rangle \]  

(52)

Therefore, after multiplying to the left by \( \hat{U}^\dagger \) and having in mind that \( \hat{U} \) is a unitary transformation

\[ \hat{H} \hat{U}^\dagger | n^o \rangle = \varepsilon_n \hat{U}^\dagger | n^o \rangle \]  

(53)

where \( \hat{U}^\dagger | n^o \rangle \) is the new eigenket of \( \hat{H} \).

Briefly, imposing the condition given by Eq. 4.7 we have the following scheme:

\[
\begin{aligned}
|n\rangle &= \hat{U}^\dagger | n^o \rangle \\
\varepsilon_n &= \varepsilon_n^o + \langle n^o | \hat{W} | n^o \rangle
\end{aligned}
\]  

(54)

That is to say, resolving the eigenvalue problem for the Hamiltonian \( \hat{H} \) implies to find the transformation \( \hat{U}^\dagger \) that makes possible the Eq. 4.7 which in turns, will allow us to write the explicit form of \( \hat{W} \).

Let us suppose now that the unitary transformation may be written as the exponential of a certain antihermitian operator, \( \hat{G} = -\hat{G}^\dagger \), henceforth referred to as the generator of the transformation. Then we immediately get, the relation

\[ \hat{W} = \hat{M} - \hat{H}^o \]

\[ \hat{W} = \hat{U} \hat{H} \hat{U}^\dagger - \hat{H}^o \]

\[ \hat{W} = \exp(\hat{G}) \hat{H} \exp(-\hat{G}) - \hat{H}^o \]  

(55)

Using the expansion of Baker-Campbell-Hausdorff [23] we get

\[ \hat{W} = \left( \hat{H} + \frac{1}{1!}[\hat{G}, \hat{H}] + \frac{1}{2!}[\hat{G}, [\hat{G}, \hat{H}]] + \cdots \right) - \hat{H}^o \]  

(56)
From Eq. 4.1 we arrive at

\[ \hat{W} = \lambda \hat{V} + \frac{1}{1!} [\hat{G}, \hat{H}^\circ + \lambda \hat{V}] + \frac{1}{2!} [\hat{G}, [\hat{G}, \hat{H}^\circ + \lambda \hat{V}]] + \cdots \]  \hspace{1cm} (57)

Let us now assume that

\[ \hat{W} = \lambda \hat{W}_1 + \lambda^2 \hat{W}_2 + \cdots \]  \hspace{1cm} (58)

and

\[ \hat{G} = \lambda \hat{G}_1 + \lambda^2 \hat{G}_2 + \cdots \]  \hspace{1cm} (59)

Insertion of Eq. 4.15 and 4.16. in Eq. 4.13, furthermore, developing, rearranging and comparing equal powers in \( \lambda \), lead us in a straightforward way to

\[ [\hat{H}^\circ, \hat{G}_1] = \hat{V} - \hat{W}_1 \]  \hspace{1cm} (60)

\[ [\hat{H}^\circ, \hat{G}_2] = \frac{1}{1!} [\hat{G}_1, \hat{V}] + \frac{1}{2!} [\hat{G}_1, [\hat{G}_1, \hat{H}^\circ]] - \hat{W}_2 \]  \hspace{1cm} (61)

\[ [\hat{H}^\circ, \hat{G}_3] = \frac{1}{1!} [\hat{G}_2, \hat{V}] + \frac{1}{2!} [\hat{G}_2, [\hat{G}_1, \hat{H}^\circ]] + \frac{1}{2!} [\hat{G}_2, [\hat{G}_2, \hat{H}^\circ]] + \frac{1}{2!} [\hat{G}_2, [\hat{G}_1, \hat{H}^\circ]] + \frac{1}{2!} [\hat{G}_1, [\hat{G}_1, \hat{H}^\circ]] - \hat{W}_3 \]  \hspace{1cm} (62)

... an so on.

It is apparent that the set of last Eqs. 4.18-4.20 is a system of coupled commutator equations for the \( \hat{G}_n \) operators. This set obeys the general structure

\[ [\hat{H}^\circ, \hat{G}_n] = \hat{A}_n - \hat{W}_n \]  \hspace{1cm} (63)

where \( \hat{H}^\circ \) and \( \hat{A}_1 = \hat{V} \), constitute the data of the problem and the \( \hat{G}_n \) are the unknown operators to be determined. The \( \hat{A}_n \) operators, with \( n \neq 1 \), are specified in terms of \( \hat{H}^\circ \) and \( \hat{A}_m \) with \( m < n \).

It is necessary to determine the \( \hat{W} \) operator, provided that \( [\hat{H}^\circ, \hat{W}] = \hat{0} \) or equivalently to that of \( \Pi(\hat{W}) = \hat{W} \). However, these conditions are fulfilled
if, in turn each one of $\hat{W}_n$ results to be a parallel component operator relative to $\hat{H}^\circ$. On this basis it may be concluded that

$$\Pi(\hat{W}_n) = \hat{W}_n$$

(64)

Now the operation with $\Pi$ on Eq. 4.21 leads to

$$\Pi([\hat{H}^\circ, \hat{G}_n]) = \Pi(\hat{A}_n) - \Pi(\hat{W}_n)$$

(65)

Having in mind the identity

$$\Pi([\hat{H}^\circ, \hat{G}_n]) = \hat{0}$$

(66)

we get

$$\Pi(\hat{A}_n) = \Pi(\hat{W}_n)$$

(67)

Thus from Eq. 4.22 we write

$$\hat{W}_n = \Pi(\hat{A}_n)$$

(68)

Otherwise, from the definition 2 we have that

$$\Gamma(\hat{G}_n) = [\hat{H}^\circ, \hat{G}_n]$$

(69)

provided that $\hat{G}_n \in \mathcal{T}_\perp$, for every $n$. However, this condition is equivalent to say that

$$\Pi(\hat{G}_n) = \hat{0}$$

(70)

Therefore from Eq. 4.22 we obtain

$$\Gamma(\hat{G}_n) = \hat{A}_n - \hat{W}_n$$

(71)

or

$$\Gamma(\hat{G}_n) = \hat{A}_n - \Pi(\hat{A}_n)$$

(72)

But the hand right side of the above equation is an operator that belongs to $\mathcal{T}_\perp$, therefore $\Gamma$ is well-defined. Thus, it may be deduced that $\Gamma^{-1}$ exists, in brief
\[ \Gamma^{-1}(\Gamma(\hat{G}_n)) = \Gamma^{-1}(\hat{A}_n - \Pi(\hat{A}_n)) \] (73)

or

\[ \hat{G}_n = \Gamma^{-1}(\hat{A}_n - \Pi(\hat{A}_n)) \] (74)

To sum up, given a problem of the type

\[ \hat{H} = \hat{H}_o + \hat{V} \] (75)

we will have that

\[ \varepsilon_n = \varepsilon_n^o + \langle n^o|\hat{W}|n^o \rangle \] (76)

and

\[ |n\rangle = \hat{U}^\dagger |n^o\rangle \] (77)

Where

\[ \hat{W} = \lambda \hat{W}_1 + \lambda^2 \hat{W}_2 + \cdots \] (78)

\[ \hat{W}_n = \Pi(\hat{A}_n) \] (79)

and

\[ \hat{G} = \lambda \hat{G}_1 + \lambda^2 \hat{G}_2 + \cdots \] (80)

\[ \hat{G}_n = \Gamma^{-1}(\hat{A}_n - \Pi(\hat{A}_n)) \] (81)

The explicit forms of any \( \hat{A}_n \) are:

\[ \hat{A}_1 = \hat{V} \] (82)

\[ \hat{A}_2 = \frac{1}{1!}[\hat{G}_1, \hat{V}] + \frac{1}{2!}[\hat{G}_1, [\hat{G}_1, \hat{H}_o]] \] (83)

16
\[ \hat{A}_3 = \frac{1}{1!} [\hat{G}_2, \hat{V}] + \frac{1}{2!} \{ \hat{G}_1, [\hat{G}_2, \hat{H}^\circ] \} + \frac{1}{2!} [\hat{G}_2, [\hat{G}_1, \hat{H}^\circ]] \]

\[ + \frac{1}{2!} [\hat{G}_1, [\hat{G}_1, \hat{V}^\circ]] + \frac{1}{3!} [\hat{G}_1, [\hat{G}_1, [\hat{G}_1, \hat{H}^\circ]]] \]

\( \cdots \) ... an so on.

In order to know all the terms of the series, we have developed a mnemonic method (Cf. appendix):

\[ \hat{A}_1 = (1) \]

\[ \hat{A}_2 = (1|1) \oplus (1, 1|0) \]

\[ \hat{A}_3 = (2|1) \oplus (1, 2|0) \oplus (2, 1|0) \oplus (1, 1|1) \oplus (1, 1|0) \]

### 5 SUMMARY AND DISCUSSIONS

It has been shown that from the spectral resolution of \( \hat{H}^\circ \), the abstract ladder operators \( \hat{\eta}_+ \) and \( \hat{\eta}_- \) may be defined. In turn, these operators serve to build multilinear operators in normal ordering \( \hat{\eta}_m^+ \hat{\eta}_n^- \). Taking advantage of the properties of the \( \hat{\eta}_m^+ \hat{\eta}_n^- \) in relation to \( \hat{H}^\circ \), we have been able to split the entire space \( \mathcal{T} \) into two subspaces \( \mathcal{T}_\parallel \) and \( \mathcal{T}_\perp \) accordingly to any operator that commutes or not with \( \hat{H}^\circ \). The above splitting of \( \mathcal{T} \) has allowed us to demonstrate the existence and uniqueness of \( \Gamma^{-1} \) under the condition that the domain and the range of \( \Gamma \) must be the orthogonal subspace \( \mathcal{T}_\perp \subset \mathcal{T} \).

Primas [7] was prevented from demonstrating this relevant theorem, because he had considered that the superoperator \( \Gamma^{-1} \) has the whole operator space \( \mathcal{T} \) as its domain.

As may be seen from Sect. 4, the entire algebraic formulation of the operator perturbation method lean heavily on the well-defined \( \Pi(\hat{\eta}_m^+ \hat{\eta}_n^-) \), \( \Gamma(\hat{\eta}_m^+ \hat{\eta}_n^-) \), and \( \Gamma^{-1}(\hat{\eta}_m^+ \hat{\eta}_n^-) \) operators.

As was remarked at the beginning, the present approach has been built independently on whatever matricial representation. Therefore, the Hamiltonian \( \hat{H}^\circ \) may have any degeneracy, however this situation is immaterial in that concern the purely algebraic relations between the operators involved.
In Part 2 of this series, the method is successfully applied to two quantum mechanical systems: “The Stark Effect in the Harmonic Oscillator” and “The Generalized Zeeman Effect”.

6 APPENDIX

In order to write out efficiently the explicit form of the commutator equations determining the \( \hat{A}_n \) operators, we have developed a mnemonic method.

RULE 1: A bracket of two sides is drawn
\[
(\cdots | \cdots)
\]

RULE 2: In the right side we must put 1 or 0.

RULE 3: In left side of the bracket we must put integers, in such way that its sum must be \( n \), i.e. the order of the iteration, consequently the subindex of \( \hat{A}_n \) superoperator.

RULE 4: We return to rule 1 until exhausting the possibilities of generating further diagrams.

RULE 5: In order to write an explicit commutator form for each operator \( \hat{A}_n \), we must consider

| Left Side | Right Side |
|-----------|------------|
| 1 \( \rightarrow \hat{G}_1 \) | 0 \( \rightarrow \hat{H}^\circ \) |
| 2 \( \rightarrow \hat{G}_2 \) | 1 \( \rightarrow \hat{V} \) |
| 3 \( \rightarrow \hat{G}_3 \) | |
| \( \ldots \) | |

Besides, we have to remember that each expression is divided by the factorial of the number of integers in left side.

As an example we calculate \( \hat{A}_2 \) and \( \hat{A}_3 \):

\[
\hat{A}_2 = (1|1) \oplus (1,1|0)
\]

\[
\hat{A}_2 = \frac{1}{1!}[\hat{G}_1, \hat{V}] + \frac{1}{2!}[\hat{G}_1, [\hat{G}_1, \hat{H}^\circ]]
\]

\[
\hat{A}_3 = (2|1) \oplus (1,2|0) \oplus (2,1|0) \oplus (1,1|1) \oplus (1,1,1|0)
\]
\[ \hat{A}_3 = \frac{1}{2!} \{ \hat{G}_2, \hat{V} \} + \frac{1}{2!} \{ \hat{G}_1, \{ \hat{G}_2, \hat{H}^\circ \} \} + \frac{1}{2!} \{ \hat{G}_1, [\hat{G}_2, \hat{H}^\circ] \} + \frac{1}{2!} \{ \hat{G}_1, [\hat{V}, \hat{G}_2] \} + \frac{1}{2!} \{ \hat{G}_1, [\hat{G}_1, \hat{H}^\circ] \} \]

In what follows we display some diagrams:

\[ \hat{A}_1 = (1) \]

\[ \hat{A}_2 = (1|1) \oplus (1,1|0) \]

\[ \hat{A}_3 = (2|1) \oplus (1,2|0) \oplus (2,1|0) \oplus (1,1|1) \oplus (1,1,1|0) \]

\[ \hat{A}_4 = (3|1) \oplus (1,3|0) \oplus (3,1|0) \oplus (2,2|0) \oplus (1,2,1) \oplus (2,1|1) \oplus (1,1,2|0) \oplus (1,2,1|0) \oplus (2,1,1|0) \oplus (1,1,1|1) \oplus (1,1,1,1|0) \]

7 ACKNOWLEDGMENTS

We thank to Miss Paula J. Espinosa M. and Mrs. A. Hasbún for subsequent helps and for reading the manuscript.

One of us (A.W.E.M.) is grateful for financial support under FONDECYT grants 1989-0657.

8 REFERENCES

References

[1] E. Schrödinger, Ann. Phys. 80, 437 (1926).

[2] P. O. Löwdin, Perturbation Theory and its Applications in Quantum Mechanics, ed. by C. H. Wilcox (Wiley, 1966).
[3] P. O. Löwdin, J. Math. Phys. 3, 969 (1962); Adv. Phys. 5, 1 (1956).

[4] J. O. Hirschfelder, Int. J. Quantum Chem. 3, 731 (1969).

[5] P. A. M. Dirac, *The Principles of Quantum Mechanics* (Clarendon Press, Oxford, 1959).

[6] J. H. Van Vleck, Phys. Rev. 33, 467 (1929); O. M. Jordal Phys. Rev. 45, 87 (1934).

[7] H. Primas, Rev. Mod. Phys. 35, 710 (1963); Helv. Phys. Acta 34, 331 (1961).

[8] F. Jørgensen, Mol. Phys. 29, 1137 (1975); F. Jørgensen and T. Pedersen, Mol. Phys. 27, 33 (1974); 27, 959 (1974).

[9] R. K. Moitra, D. Mukherjee and A. M. Pramana 9, 545 (1977); Mol. Phys. 30, 1961 (1975); 33, 953 (1977).

[10] P. Westhans, E. G. Bradford and D. Hall, J. Chem. Phys. 62, 1607 (1975); P. Westhaus, Int. J. Quantum Chem. 20, 1243 (1981).

[11] T. Kato, Prog. Theor. Phys. 4, 514 (1959); C. Bloch and J. Horowitz, Nucl. Phys. 8, 91 (1958); B. H. Brandow, Rev. Mod. Phys. 39, 771 (1967).

[12] L. De la Peña and R. Montemayor, Am. J. Phys. 48, 855 (1980).

[13] F.M. Fernández and E. A. Castro, Am. J. Phys. 52, 344 (1984).

[14] J. Cizek and J. Paldus, Int. J. Quantum Chem. 12, 875 (1977).

[15] M. Berrondo and A. Palma, J. Phys. A: Math. Gen. 13, 773 (1980).

[16] J. Morales, J. López-Bonilla and A. Palma, J. Math. Phys. 28, 1032 (1987).

[17] N. W. Bazley and D. W. Fox, Rev. Mod. Phys. 35, 712 (1963).

[18] P. O. Löwdin, Int. J. Quantum Chem. 16, 485 (1982).
[19] J. A. Crawford, Nuovo Cimento 10, 698 (1958); M. Rosenblum, Duke Math. J. 23, 263 (1956).

[20] F. J. Murray, J. Math. Phys. 3, 451 (1962).

[21] S. Lang, Linear Algebra (Wesley, 1971).

[22] M. Schechter, Operatorial Methods in Quantum Mechanics (North Holland, 1981).

[23] F. Hausdorff, Leipziger Ber. Ges. Wiss. Math. Phys. kl. 58, 19 (1906).