ALGEBRAIC FORMULATION OF THE OPERATORIAL PERTURBATION THEORY. PART 2. APPLICATIONS

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Abstract

The algebraic approach to operator perturbation method has been applied to two quantum–mechanical systems “The Stark Effect in the Harmonic Oscillator” and “The Generalized Zeeman Effect”. To that end, two realizations of the superoperators involved in the formalism have been carried out. The first of them has been based on the Heisenberg–Dirac algebra of $\hat{a}^\dagger$, $\hat{a}$, $\hat{1}$ operators, the second one has been based in the angular momentum algebra of $\hat{L}_+$, $\hat{L}_-$ and $\hat{L}_0$ operators. The successful results achieved in predicting the discrete spectra of both systems have put in evidence the reliability and accuracy of the theory.
1 Introduction

The principal aim of this paper is to present how easily the algebraic approach to perturbation methods developed in Part 1 of this series works.

The practice of ladder operators in the Operator Perturbation Method have led to general lemmas that make easier the applications of the present Algebraic Formulation of the Operator Perturbation Theory (AFOPT) to non–relativistic quantum mechanics. A fruitful procedure is to write the parallel projection superoperator $\Pi$, the derivation superoperator $\Gamma$ and its inverse $\Gamma^{-1}$ in terms of the ladder operators of a given algebra associated with the physics of the problem at hands. This algebraic approach to operator perturbation method can be applied, in principle, to any problem provided that one can build the explicit and proper form of the ladder operator common to $\hat{H}^0$ and the perturbation $\hat{V}$.

The paper is arranged as follows: in order to study the first system, i.e. a charged harmonic oscillator the $\hat{a}^\dagger$, $\hat{a}$ and $\hat{1}$, ladder operators of the Heisenberg–Dirac algebra has been introduced in Sect. 2. Then, we recover the $\Pi$, $\Gamma$ and $\Gamma^{-1}$ superoperators in terms of the before mentioned ladder operators. To study the second system, this time the Generalized Zeeman Effect, the spherical base of angular momentum operators $\hat{L}_+$, $\hat{L}_-$ and $\hat{L}_z$ have been introduced in Sect. 2.1. Here we retrieve the aforementioned set of superoperators, now in terms of the ladder operators associated with the angular momentum algebra.

In Sect. 2.2 and 3 all the machinery developed in Part 1 of this series has been totally applied to both quantum mechanical systems.

In the last Sect. 4 the paper concludes with a general discussion high-lightening the reliability and accomplishment of the theory.

2 The Stark Effect in the Harmonic Oscillator

Let us consider a particle of charge $e$ and mass $m$, oscillating about its equilibrium position, with fundamental frequency $\omega_0$, subjects to a homogeneous electric field of strength $E$. We assume that the oscillations are parallel to the direction of field.
The full Hamiltonian \( \hat{H} \) is split into a zero order Hamiltonian \( \hat{H}^0 \) and a perturbation \( \hat{V} \)

\[
\hat{H} = \hat{H}^0 + \lambda \hat{V} \quad \lambda \in [0, 1]
\]

Next we introduce the raising and lowering operators \( \hat{a}^\dagger \) and \( \hat{a} \) through the usual canonical transformation

\[
\hat{q} = \sqrt{\frac{\hbar}{2m\omega_0}} (\hat{a}^\dagger + \hat{a}) \\
\hat{p} = i \sqrt{\frac{\hbar m\omega_0}{2}} (\hat{a}^\dagger - \hat{a})
\]

with

\[
[\hat{a}^\dagger, \hat{a}] = 1
\]

As it is well–known, the zero order Hamiltonian may now be written as

\[
\hat{H}^0 = (\hat{a}^\dagger \hat{a} + \frac{1}{2} \hat{1}) \hbar \omega_0.
\]

The perturbation operator is

\[
\hat{V} = -eE\hat{q} = -eE \sqrt{\frac{\hbar}{2m\omega_0}} (\hat{a}^\dagger + \hat{a})
\]

Here \( \hat{q} \) is the position operator of the particle regarding its equilibrium position. The electric field strength plays the role of the perturbation parameter \( \lambda \). Hence, when the perturbation is switched on, the zero order eigenkets \( |n^0\rangle \) evolve into orthogonal perturbed eigenkets \( |n\rangle \) of energy \( \varepsilon_n \). Then from Part 1 we may write

\[
|n\rangle = \hat{U}^\dagger |n^0\rangle
\]

and

\[
\varepsilon_n = \varepsilon_n^0 + \langle n^0 | \hat{W} | n^0 \rangle
\]
Resolving the eigenvalue problem for the full Hamiltonian $\hat{H}$ involves to find the unitary transformation $\hat{U} = \exp(\hat{G})$, which must fulfill the requirement

$$[\hat{H}, \hat{W}] = 0$$

The unitary transformation will allow us to find the explicit form of the $\hat{W}$ operator [1].

From Part 1, it can be seen that three superoperators are of special importance to algebraic formulation of the perturbation method. In fact, from the following equations

$$\hat{W} = \sum_n \hat{W}_n , \quad \hat{W}_n = \Pi(\hat{A}_n)$$  \hspace{1cm} (1)

and

$$\hat{G} = \sum_n \hat{G}_n , \quad \hat{G}_n = \Gamma^{-1}(\hat{A}_n - \Pi(\hat{A}_n))$$  \hspace{1cm} (2)

it is apparent that $\Pi$, $\Gamma$ and $\Gamma^{-1}$ are such superoperators.

2.1 Expressions for $\Pi$, $\Gamma$ and $\Gamma^{-1}$ superoperators in terms of $\hat{a}^\dagger$ and $\hat{a}$ ladder operators

We look now at a representation of the superoperator $\Pi$, $\Gamma$ and $\Gamma^{-1}$ in terms of raising and lowering operators $\hat{a}^\dagger$ and $\hat{a}$. The straightforward application of the method outlined in Sect. 3 of Part 1, allows us to write for the $\Pi$ superoperator, the algebraic form

$$\Pi(\hat{a}^\dagger m \hat{a}^n) = \delta_{mn} \hat{a}^\dagger m \hat{a}^n$$  \hspace{1cm} (3)

Analogously the same reference of Part 1, leads us to write for the $\Gamma$ superoperator the expression

$$\Gamma(\hat{a}^\dagger m \hat{a}^n) = (m - n) \hbar \omega_0 \hat{a}^\dagger m \hat{a}^n$$

Finally, from the well-defined $\Gamma^{-1}$ superoperator we may write
\[
\Gamma^{-1}(\hat{a}^m \hat{a}^n) = \begin{cases} 
\hat{0} & \text{if } m = n \\
\frac{(m-n)\hbar\omega_0}{\hbar} \hat{a}^m \hat{a}^n & \text{if } m \neq n 
\end{cases} \tag{4}
\]

Notice that the integers \( m, n \) do not label the energy level, really they label the powers of \( \hat{a}^\dagger \) and \( \hat{a} \) in the multilinear operator \( \hat{a}^m \hat{a}^n \).

### 2.2 Solution of the Perturbation Equations

According to Eqs. 1 and 2 the solution of the perturbation equations implies to find the \( \hat{A}_n \) operators, which in turn are determined through the commutator equation in terms of \( \hat{H}^0, \hat{V} \) and the \( \hat{G}_m, m < n \) operators.

From the mnemonic box diagrams given in the appendix of Part 1 the explicit form of the commutator equations, follow straightforwardly.

#### 2.2.1 First Iteration

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

\[
\hat{W}_1 = \Pi \left( \hat{V} \right) = -e\sqrt{\frac{\hbar}{2m\omega_0}} \Pi (\hat{a}^\dagger + \hat{a})
\]

But according to Eq. \( 3 \) follows

\[
\Pi (\hat{a}^\dagger) = \hat{0} \quad \text{and} \quad \Pi (\hat{a}) = \hat{0}
\]

Thus

\[
\hat{W}_1 = \Pi (\hat{A}_1) = \hat{0}
\]

Now we must calculate \( \hat{G}_1 \).
\[
\hat{G}_1 = \Gamma^{-1} (\hat{A}_1 - \Pi (\hat{A}_1)) \\
= \Gamma^{-1} (\hat{A}_1) \\
= -eE \sqrt{\frac{\hbar}{2m\omega_0}} \Gamma^{-1} (\hat{a}^\dagger + \hat{a})
\]

From Eq. 4 we have

\[
\Gamma^{-1} (\hat{a}^\dagger) = (\hbar \omega_0)^{-1} \hat{a}^\dagger
\]

and

\[
\Gamma^{-1} (\hat{a}) = (\hbar \omega_0)^{-1} \hat{a}
\]

Altogether, we may write

\[
\hat{G}_1 = -eE \sqrt{\frac{\hbar}{2m\omega_0}} (\hat{a}^\dagger + \hat{a})
\]

### 2.2.2 Second Iteration

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

Having in mind the rules of box diagrams of Part 1 we may write down

\[
\hat{A}_2 = \frac{1}{1!} [\hat{G}_1, \hat{V}] + \frac{1}{2!} [\hat{G}_1, [\hat{G}_1, \hat{H}^0]]
\]

The evaluation of this commutators is straightforward, thus we have

\[
[\hat{G}_1, \hat{V}] = -\frac{e^2 \mathcal{E}^2}{m\omega_0^2} \hat{1}
\]

\[
[\hat{G}_1, [\hat{G}_1, \hat{H}^0]] = \frac{e^2 \mathcal{E}^2}{m\omega_0^2} \hat{1}
\]

Therefore
Since $\Pi(\text{cte}) = \text{cte}$, we get

$$\hat{W}_2 = \Pi(\hat{A}_2) = -\frac{1}{2} \left( \frac{e^2 \mathcal{E}^2}{m \omega_0^2} \right) \hat{1}$$

and it is immediate that

$$\hat{G}_2 = \Gamma^{-1} \left( \hat{A}_2 - \Pi(\hat{A}_2) \right) = \hat{0}$$

### 2.2.3 Higher Iterations

Proceeding with higher iterations it is easy to see that the $\hat{A}_3, \hat{A}_4, \ldots$ operators are all null, since $\hat{G}_2 = \hat{0}$.

Finally, from Eqs. 1, 2 we obtain

$$\hat{W} = -\frac{1}{2} m \left( \frac{e \mathcal{E}}{m \omega_0} \right)^2 \hat{1}$$

and

$$\hat{G} = \frac{i}{\hbar} \frac{e \mathcal{E}}{m \omega_0^2} \hat{p}$$

To sum up, the energies and the eigenvectors of the full Hamiltonian become

$$\varepsilon_n = \varepsilon_n^0 - \frac{1}{2} m \left( \frac{e \mathcal{E}}{m \omega_0} \right)^2$$

and

$$|n\rangle = \exp \left( -\frac{i}{\hbar} \frac{e \mathcal{E}}{m \omega_0^2} \hat{p} \right) |n^0\rangle$$

These results exactly coincide with those known from the elementary courses of quantum mechanics. They show the reliability and accuracy of the calculations achieved with our algebraic formulation of the operator perturbation theory.
3 Generalized Zeeman Effect

To study this quantum mechanical system we will introduce the algebra of angular momentum operator. But instead of working with cartesian component operators $\hat{L}_x$, $\hat{L}_y$ and $\hat{L}_z$, it will be more convenient for the algebraic formalism to use the spherical representation defined by

$$\hat{L}_+ = \hat{L}_x + i\hat{L}_y$$

$$\hat{L}_- = \hat{L}_x - i\hat{L}_y$$

$$\hat{L}_0 = \hat{L}_z$$

Where the $\hat{L}_+$ and $\hat{L}_-$ are the raising and lowering angular momentum operators. For the sake of completeness we add the well–known relation: $\hat{L}^2 = \hat{L}_x^2 + \hat{L}_y^2 + \hat{L}_z^2$, which satisfies the fundamental commutator

$$[\hat{L}_z, \hat{L}_z] = 0$$

where from the two distinguished relations follow

$$\hat{L}^2 |lm\rangle = l(l + 1)\hbar^2 |lm\rangle$$

and

$$\hat{L}_z |lm\rangle = m\hbar |lm\rangle .$$

The $|lm\rangle$ will define the zero–order orthonormal eigenkets $|lm\rangle$, a base whereon to build the orthonormal eigenkets $|lm\rangle$.

Now we will inquire about the representation of $\Pi$, $\Gamma$ and $\Gamma^{-1}$ in terms of the angular spherical operators, $\hat{L}_+$, $\hat{L}_-$ and $\hat{L}_0$.

Prior to tackle this problem we want to state the next result, easily to prove by mathematical induction the 0-component operator $\hat{L}_0$ and the multilinear operator $\hat{L}_+^m \hat{L}_0^p \hat{L}_-^n$, which satisfies the following commutator relation

$$[\hat{L}_z, \hat{L}_+^m \hat{L}_0^p \hat{L}_-^n] = (m - n) \hbar \hat{L}_+^m \hat{L}_0^p \hat{L}_-^n$$

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The system is a hydrogen atom exposed to two constant uniform magnetic fields: one of them is parallel to the $z$–axis and the other lies in the $(x, y)$–plane perpendicular to the $z$–axis.

The full Hamiltonian of such system is

\[ \hat{H} = \hat{H}^0 + \hat{V} \]

where the unperturbed Hamiltonian is

\[ \hat{H}^0 = \hat{H}^0_R + \frac{\alpha}{r^2} \hat{L}^2 + \kappa \hat{L}_z \]

here $\hat{H}^0_R$ is a radial Hamiltonian, $\alpha$ and $\kappa$ are positive constants. The perturbation operator is

\[ \hat{V} = a \hat{L}_x + b \hat{L}_y \]

The real parameters $a$ and $b$ satisfy the normalization condition

\[ a^2 + b^2 = 1 \]

Along the same line of reasoning outlined in Part 1, we state now the following expressions for $\Pi$, $\Gamma$ and $\Gamma^{-1}$ superoperators in terms of the spherical base of operators

\[ \Pi \left( \hat{L}_m^p \hat{L}_n^p \hat{L}_n^p \right) = \delta_{mn} \hat{L}_m^p \hat{L}_n^p \hat{L}_n^p \quad (5) \]

\[ \Gamma \left( \hat{L}_m^p \hat{L}_n^p \hat{L}_n^p \right) = (m - n) \hbar \kappa \hat{L}_m^p \hat{L}_n^p \hat{L}_n^p \]

Furthermore, since the superoperator $\Gamma^{-1}$ is well–defined we get

\[ \Gamma^{-1} \left( \hat{L}_m^p \hat{L}_n^p \hat{L}_n^p \right) = \begin{cases} \hat{0} & \text{if } m = n \\ [(m - n) \hbar \kappa]^{-1} \hat{L}_m^p \hat{L}_n^p \hat{L}_n^p & \text{if } m \neq n \end{cases} \]

It is relevant to remark that the above realization is independent of any degeneracy of the Hamiltonian [1] and the magnitude of the perturbation is also immaterial [3].
It is convenient for further calculations to transform the perturbation operator. Since:

\[
\hat{L}_x = 2 \left( \hat{L}_+ + \hat{L}_- \right) \quad \text{and} \quad \hat{L}_x = \frac{i}{2} \left( \hat{L}_+ - \hat{L}_- \right)
\]

We write

\[
\hat{V} = \frac{1}{2} (a + ib) \hat{L}_+ + \frac{1}{2} (a - ib) \hat{L}_-
\]

with \(u = a + ib\) we have

\[
\hat{V} = \frac{1}{2} u \hat{L}_+ + \frac{1}{2} u^* \hat{L}_-
\]

and

\[|u|^2 = 1.\]

### 3.1 Solution of the Perturbation Equation

The zero–order eigenenergies suitable to the \(\hat{H}^0\) Hamiltonian are given by

\[\varepsilon_{lm}^0 = \varepsilon_{lm}^0 + \frac{\alpha}{r^2} l (l + 1) \hbar^2 + m \hbar \kappa.\]

The eigenenergies of the respective perturbed Hamiltonian are

\[\varepsilon_{lm} = \varepsilon_{lm}^0 + \langle lm | \hat{W} | lm \rangle\]

and the orthonormal eigenkets are

\[|lm\rangle = \exp \left( -\hat{G} \right) |lm\rangle\]

Also we note from Part 1 that

\[\hat{W} = \sum_n \hat{W}_n \quad n = 1, 2, \ldots\]

and

\[\hat{G} = \sum_n \hat{G}_n \quad n = 1, 2, \ldots\]

where

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

and

\[\hat{G}_n = \Gamma^{-1} \left( \hat{A}_n - \Pi \left( \hat{A}_n \right) \right)\]
3.1.1 First Iteration

\[ \hat{A}_1 = (1) = \hat{V} = \frac{1}{2} u \hat{L}_+ + \frac{1}{2} u^* \hat{L}_- \]

then

\[ \hat{W}_1 = \Pi (\hat{A}_1) = \frac{1}{2} u \Pi (\hat{L}_+) + \frac{1}{2} u^* \Pi (\hat{L}_-) \]

Therefore from Eq. 3 we conclude that

\[ \hat{W}_1 = 0 \]

Furthermore,

\[ \hat{G}_1 = \Gamma^{-1} (\hat{A}_1) \]

\[ = \frac{1}{2} u \left( \frac{1}{\hbar \kappa} \hat{L}_+ \right) + \frac{1}{2} u^* \left( -\frac{1}{\hbar \kappa} \hat{L}_- \right) \]

\[ = \frac{1}{2 \hbar \kappa} (u \hat{L}_+ - u^* \hat{L}_-) \]

3.1.2 Second Iteration

The diagrammatic expansion for the \( \hat{A}_2 \) operator is

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

From the aforementioned rules follow

\[ \hat{A}_2 = \frac{1}{\Pi} [\hat{G}_1, \hat{V}] + \frac{1}{2!} [\hat{G}_1, [\hat{G}_1, \hat{H}^0]] \]

From the operatorial expression of \( \hat{G}_1 \) and \( \hat{V} \) it is easy to get

\[ [\hat{G}_1, \hat{V}] = \frac{1}{\kappa} \hat{L}_0 \]

For the second commutator it is profitable to remark that

\[ [\hat{G}_1, \hat{H}^0] = -\Gamma (\hat{G}_1) \]
Thus
\[ \hat{G}_1 = \Gamma^{-1} (\hat{A}_1) = \Gamma^{-1} (\hat{V}) \]

Then, left multiplying by \( \Gamma \) one obtains
\[ \hat{V} = \Gamma (\hat{G}_1) \]

In all we may write
\[ \frac{1}{2!} [\hat{G}_1, [\hat{G}_1, \hat{H}^0]] = -\frac{1}{2} [\hat{G}_1, \hat{V}] = -\frac{1}{2\kappa} \hat{L}_0 \]

In short, the \( \hat{A}_2 \) operator is
\[ \hat{A}_2 = \frac{1}{\kappa} \hat{L}_0 - \frac{1}{2\kappa} \hat{L}_0 = \frac{1}{2\kappa} \hat{L}_0 \]

The \( \hat{G}_2 \) operator is
\[ \hat{G}_2 = \Gamma^{-1} (\hat{A}_2) = \frac{1}{2\kappa} \Gamma^{-1} (\hat{L}_0) \]

However from Eq. 4 \( m = n = 0 \), then it follows that
\[ \hat{G}_2 = 0 \]

Hence any commutator involving \( \hat{G}_2 \) must be vanished. Therefore it can be concluded that in the third iteration the only non null commutator leads to the equation
\[ \hat{A}_3 = \frac{1}{2!} [\hat{G}_1, [\hat{G}_1, \hat{H}^0]] + \frac{1}{3!} [\hat{G}_1, [\hat{G}_1, [\hat{G}_1, \hat{H}^0]]] \]

### 3.1.3 Third Iteration

A straightforward calculation gives
\[ \hat{A}_3 = -\frac{1}{3\kappa^2} \hat{V} \]

Here it is easy to check that
\[ \hat{W}_3 = 0 \]

and
\[ \hat{G}_3 = -\frac{1}{3\kappa^2} \hat{G}_1 \]
3.1.4 Fourth Iteration

Alongside the same calculation we arrive to

\[ \hat{A}_4 = -\frac{1}{8\kappa^3} \hat{L}_0 \]

Then

\[ \hat{W}_4 = -\frac{1}{8\kappa^3} \hat{L}_0 \]

and

\[ \hat{G}_4 = 0 \]

From the expansion given by Eq. 1 and Eq. 2, one arrives to

\[ \hat{G} = \left( \frac{1}{\kappa} - \frac{1}{3\kappa^2} + \cdots \right) (u\hat{L}_+ - u^*\hat{L}_-) \]

and

\[ \hat{W} = \left( \frac{1}{2\kappa} - \frac{1}{8\kappa^3} + \cdots \right) \hat{L}_0 \]

From the above results we can say that our algebraic calculations are coincident with those early reported by Arthurs and Robinson [4].

4 Summary and Discussions

In order to show the subsequent stages involved in our calculations of the discrete spectra of quantum mechanical systems, two systems have been chosen: “The Stark Effect in the Harmonic Oscillator” and “The Generalized Zeeman Effect”. These systems have been studied with greater details throughout so as to show how the present algebraic formalism works.

The sharp coincidence of the results so obtained confirms the reliability and easiness of the calculations involved.

Another aspect of the method is the internal coherency and self consistency. In other words it has not been necessary to introduce any unconnected
elements with the theory, as well as trials and errors assays in order to carry out the calculations of the spectra of both systems.

Finally some practical consequences may be drawn from the performed algebraic operations. Sometimes the commutator equations of higher orders seem to be very involved and tiresome. However, just a bit of systematic work on this kind of equations reveals that many expressions have already been calculated or an unknown quantity may be written in terms of another quantity already calculated.

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