Alternative analysis to perturbation theory

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We develop an alternative approach to time independent perturbation theory in non-relativistic quantum mechanics. The method developed has the advantage to provide in one operation the correction to the energy and to the wave function, additionally we can analyze the time evolution of the system. To verify our results, we apply our method to the harmonic oscillator perturbed by a quadratic potential. An alternative form of the Dyson series, in matrix form instead of integral form, is also obtained.

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I. INTRODUCTION

The Schrödinger equation is the main equation in non-relativistic quantum mechanics. Although it has been widely studied since its introduction, there are only few cases in which it can be solved exactly. Typical examples of potentials where an exact analytical solution is known, are the infinite well, the harmonic oscillator, the hydrogen atom, and the Morse potential. The great majority of the problems related with the Schrödinger equation are very complex and can not be solved exactly, as is the case of the cosine potential for instance. When an exact analytical solution can not be found, we are forced to apply approximation methods, that when correctly used, give us a very good understanding of the behavior of the quantum system. For the sake of clarity, we will briefly revise one of those methods: the time independent perturbation theory, also known as Rayleigh-Schrödinger perturbation theory. This method has its roots in the works of Rayleigh and Schrödinger, but the mathematical foundations were only set by Rellich in the late thirties of the past century (see Simon and references there in). This method has been applied with great success to solve a vast variety of problems such that, through its continuous implementation, a lot of techniques have been developed, which go from numerical methods to those more mathematical and fundamental, as convergency problems. The Rayleigh-Schrödinger theory is appropriate when we have a time independent Hamiltonian, that can be separated in two parts, as follows:

\[ \hat{H} = \hat{H}_0 + \hat{H}_p, \]  

where \( \hat{H}_0 \) is the so-called non-perturbed Hamiltonian, and it is usually assumed to have known solutions, this is, its eigenvalues

\[ \hat{H}_0 |n^{(0)} \rangle = E_n^{(0)} |n^{(0)} \rangle \]  

are known. The second part of the Hamiltonian, \( \hat{H}_p \), is small compared to \( \hat{H}_0 \); thus \( \hat{H}_p \) is called the "perturbation", because its effect in the energy spectrum and in the eigenfunctions will be small. To be more explicit, it is usual to write \( \hat{H}_p \) in terms of a dimensionless real parameter \( \lambda \), which is considered very small compared to one

\[ \hat{H}_p = \lambda \hat{V} \quad (\lambda \ll 1). \]  

Here, we propose an alternative perturbation method based on the evolution operator for Hamiltonian, i.e., the exponential of the complete Hamiltonian. Making use of the Taylor series of the exponential and operator techniques we will cast the solution into a form that has powers of tridiagonal matrices in it. By using as an example a perturbative potential for which we know the solutions, we will be able to compare our method with the Rayleigh-Schrödinger perturbation theory. Our method will allow also to cast the Dyson series, which are written in multiple integral forms, as a series of powers of tridiagonal matrices.

We will proceed then as follows, in section II, we present a brief summary of the standard time independent perturbation theory, emphasizing the expressions obtained for the first and second order corrections. As is well known, two expressions are obtained at each order, one for the energies and one for the wave functions. In Section III, we introduce our matrix approach to perturbation theory that will allow us to obtain a single solution that contains both, the energy and wave function corrections. We will introduce there all the corrections to the wave function that will allow us to generate later the Dyson series, and in this way give also a new expression of it but now in terms of a matrix series. In Section IV we compare the our method with the standard perturbation theory by solving the harmonic oscillator with a quadratic perturbation. Although this seems redundant, because this case has an
exact solution, it will allow us to compare both methods by doing an expansion of the exact solution in terms of the perturbation parameter, \( \lambda \). In Section V we apply our formalism to rewrite the Dyson series in matrix form and Section VI is left for conclusions.

**II. PERTURBATION THEORY**

As we already mention, we have to solve the eigenvalue problem given by (1). Standard perturbation theory produces the following expressions for the eigenvalues

\[
E_n = E_n^{(0)} + \lambda \Delta_n^{(1)} + \lambda^2 \Delta_n^{(2)} + \cdots ,
\]

and the eigenfunctions

\[
|n\rangle = |n^{(0)}\rangle + \lambda |n^{(1)}\rangle + \lambda^2 |n^{(2)}\rangle + \cdots .
\]

In the two previous equations the super index \((j)\) indicates the correction order. The first and second order corrections for the energy are

\[
\Delta_n^{(1)} = \langle n^{(0)}|\hat{V}|n^{(0)}\rangle = V_{nn} \quad (6)
\]

\[
\Delta_n^{(2)} = \langle n^{(0)}|\hat{V}|n^{(1)}\rangle = \sum_{k \neq n} \frac{|V_{kn}|^2}{E_n^{(0)} - E_k^{(0)}} \quad (7)
\]

where we have defined

\[
V_{kn} = \langle k^{(0)}|\hat{V}|n^{(0)}\rangle .
\]

For the wave functions the first two order corrections are given by the expressions

\[
|n^{(1)}\rangle = \sum_{k \neq n} \frac{|k^{(0)}\rangle V_{kn}}{E_n^{(0)} - E_k^{(0)}} \quad (9)
\]

and

\[
|n^{(2)}\rangle = \sum_{k \neq n} \sum_{m \neq n} \frac{|k^{(0)}\rangle V_{km} V_{mn}}{(E_n^{(0)} - E_k^{(0)})(E_n^{(0)} - E_m^{(0)})} - \sum_{k \neq n} \frac{|k^{(0)}\rangle V_{nn} V_{kn}}{(E_n^{(0)} - E_k^{(0)})^2} \quad (10)
\]

It is clear that the previous expressions can be used in the non-degenerate case, where we always have \( E_n^{(0)} \neq E_k^{(0)} \). In the degenerate case, a different treatment is needed.

**III. MATRIX APPROACH TO THE PERTURBATION THEORY**

**A. First order correction**

We now find an approximate solution for the complete (time dependent) Schrödinger equation; i.e., we will solve approximately the equation

\[
i \frac{\partial}{\partial t} |\psi\rangle = \hat{H} |\psi\rangle = \left( \hat{H}_0 + \lambda \hat{V} \right) |\psi\rangle .
\]

The formal solution may be written as

\[
|\psi(t)\rangle = e^{-i(\hat{H}_0 + \lambda \hat{V}) |\psi(0)\rangle} ,
\]

that by expanding the exponential in a Taylor series

\[
|\psi(t)\rangle = \sum_{n=0}^{\infty} \frac{(-it)^n}{n!} \left( \hat{H}_0 + \lambda \hat{V} \right)^n |\psi(0)\rangle ,
\]

(13)
is obtained. If we develop the binomials inside the summation, rearrange terms and cut the series to first order in \( \lambda \), we have

\[
|\psi(t)| \approx \left( \sum_{n=0}^{\infty} \frac{(-it)^n}{n!} H_0^n + \lambda \sum_{n=1}^{\infty} \frac{(-it)^n}{n!} \sum_{k=0}^{n-1} H_0^{n-1-k} \hat{V} H_0^k \right) |\psi(0)|. \tag{14}
\]

The key ingredient of the method we introduce in this contribution is the matrix

\[
M = \begin{pmatrix} \hat{H}_0 & \hat{V} \\ 0 & \hat{H}_0 \end{pmatrix}, \tag{15}
\]

It is very easy to get convinced that the following relations are satisfied

\[
(M)_{1,2} = \hat{V}, \quad (M^2)_{1,2} = \hat{H}_0 \hat{V} + \hat{V} \hat{H}_0, \quad \ldots \quad (M^n)_{1,2} = \sum_{k=0}^{n-1} H_0^{n-1-k} \hat{V} H_0^k. \tag{16}
\]

Thus, equation (14) can be written as

\[
|\psi(t)| \approx \left[ \sum_{n=0}^{\infty} \frac{(-it)^n}{n!} (\hat{H}_0^n + \lambda \sum_{n=1}^{\infty} \frac{(-it)^n}{n!} (M^n)_{(1,2)}) \right] |\psi(0)|. \tag{17}
\]

As \( M^0 = I \) (where \( I \) is the \([2 \times 2]\) identity matrix), we trivially have that

\[
(M^0)_{(1,2)} = 0,
\]

and substituting this term in equation (17) we obtain

\[
|\psi(t)| \approx \left( e^{-it\hat{H}_0} + \lambda (e^{-itM})_{(1,2)} \right) |\psi(0)| = e^{-it\hat{H}_0} |\psi(0)| + \lambda (e^{-itM})_{(1,2)} |\psi(0)|. \tag{18}
\]

Note that in the last expression we have separated the approximate solution in two parts; the first part is the solution of the non-perturbed system, that is well known, and the second part is the first order correction to the wave function. We now show how the correction to first order may be calculated, for this we rewrite equation (17) as

\[
|\psi(t)| \approx |\psi^{(0)}(t)| + \lambda (||\psi^p||)_{1,2}, \tag{19}
\]

where we have defined the matrix wave function

\[
||\psi^p|| = \begin{pmatrix} |\psi^{(1,1)}| & |\psi^{(1,2)}| \\ |\psi^{(2,1)}| & |\psi^{(2,2)}| \end{pmatrix}. \tag{20}
\]

Deriving (17) and (18) with respect to time and equating them, we arrive to the equation

\[
i \frac{\partial}{\partial t} |\psi^{(0)}(t)| + i \lambda \frac{\partial}{\partial t} (||\psi^p||)_{1,2} = \hat{H}_0 e^{-it\hat{H}_0} |\psi(0)| + \lambda (Me^{-itM} I |\psi(0)|)_{1,2}. \tag{21}
\]

Equating powers of \( \lambda \), we have

\[
i \frac{\partial}{\partial t} (||\psi^p||)_{1,2} = (Me^{-itM} I |\psi(0)|)_{1,2}. \tag{22}
\]

We have to solve now equation (21), or equivalently the system

\[
i \frac{\partial}{\partial t} \begin{pmatrix} |\psi^{(1,1)}| & |\psi^{(1,2)}| \\ |\psi^{(2,1)}| & |\psi^{(2,2)}| \end{pmatrix} = Me^{-itM} \begin{pmatrix} |\psi(0)| & 0 \\ 0 & |\psi(0)| \end{pmatrix}. \tag{23}
\]
Integrating this equation, we have
\[
||\psi^p|| = e^{-itM} \begin{pmatrix} ||\psi(0)|| & 0 \\ 0 & ||\psi(0)|| \end{pmatrix},
\]
(23)
to finally write the differential equation
\[
i \frac{\partial}{\partial t} ||\psi^p|| = M||\psi^p||,
\]
(24)
with the initial condition
\[
||\psi^p(0)|| = \begin{pmatrix} ||\psi(0)|| & 0 \\ 0 & ||\psi(0)|| \end{pmatrix}.
\]
(25)
The needed solution is associated with the second column of matrix ||\psi^p||, thus we write
\[
i \frac{\partial}{\partial t} \begin{pmatrix} \psi(1,2) \\ \psi(2,2) \end{pmatrix} = M \begin{pmatrix} \psi(1,2) \\ \psi(2,2) \end{pmatrix},
\]
but, because \(M\) is a tridiagonal matrix, the system may be directly integrated. We show it by writing explicitly
\[
i \frac{\partial}{\partial t} \psi(1,2) = \hat{H}_0 \psi(1,2) + \hat{V} e^{-i\hat{H}_0 t} \psi(0),
\]
(26)
and
\[
i \frac{\partial}{\partial t} \psi(2,2) = \hat{H}_0 \psi(2,2),
\]
(27)
with the initial condition
\[
\begin{pmatrix} 0 \\ |\psi(0)|| \end{pmatrix}.
\]
(28)
Because we know the solution for \(\hat{H}_0\), equation (27) is solved trivially,
\[
|\psi(2,2)|| = e^{-i\hat{H}_0 t} |\psi(0)||, 
\]
(29)
that substituted in (26), allows us to write
\[
i \frac{\partial}{\partial t} \psi(1,2) = \hat{H}_0 \psi(1,2) + \hat{V} e^{-i\hat{H}_0 t} \psi(0),
\]
Making the transformation \(|\psi(1,2)|| = e^{-i\hat{H}_0 t} |\phi_{1,2}(x)||\), we arrive to the equation
\[
i \frac{\partial}{\partial t} \phi_{1,2} = e^{i\hat{H}_0 t} \hat{V} e^{-i\hat{H}_0 t} |\psi(0)||
\]
that can be easily integrated to give
\[
|\phi_{1,2}|| = -i \left[ \int_0^t e^{i\hat{H}_0 t_1} \hat{V} e^{-i\hat{H}_0 t_1} dt_1 \right] |\psi(0)||,
\]
and by transforming back the solution to the first correction may be obtained
\[
|\psi_{1,2}|| = -ie^{-i\hat{H}_0 t} \int_0^t e^{i\hat{H}_0 t_1} \hat{V} e^{-i\hat{H}_0 t_1} dt_1 |\psi(0)||.
\]
(30)
Up to here we have produced a first order correction for the wave function with no assumptions on Hamiltonian degeneracy, therefore making this first order correction valid also for degenerate Hamiltonians.
As the eigenfunctions of the non-perturbed Hamiltonian constitutes a complete orthonormal set, we can write the closure condition as \( I = \sum_k |k^{(0)}\rangle \langle k^{(0)}| \), where \( |k^{(0)}\rangle \) are the eigenstates of the unperturbed Hamiltonian and insert the identity operator written in this way, in equation (30) to arrive to

\[
|\psi_{1,2}\rangle = -i \sum_k |k^{(0)}\rangle \langle k^{(0)}| e^{-iR_0 t} \left[ \int_0^t e^{iR_0 t_1} \hat{V} e^{-iR_0 t_1} dt_1 \right] |\psi(0)\rangle. \tag{31}
\]

For simplicity we set the initial condition \( |\psi(0)\rangle = |n^{(0)}\rangle \). By defining

\[
|n^{(1)}\rangle_t = \sum_{k \neq n} \frac{|k^{(0)}\rangle V_{kn}}{E^{(0)}_n - E^{(0)}_k} e^{-iE^{(0)}_k t}, \tag{32}
\]

and using expressions (6) and (9), we finally get

\[
|\psi_{1,2}\rangle = e^{-iE^{(0)}_k t} \left[ |n^{(1)}\rangle - it|n^{(0)}\rangle \Delta^{(1)} \right] - |n^{(1)}\rangle_t. \tag{33}
\]

We note that the first order corrections to the energy and to the wave function are already contained in the last expression. Additionally we can show that we can write

\[
||\psi^p\rangle = e^{-itH_0} \begin{pmatrix} 1 & -i \int_0^t dt_1 \hat{V}(t_1) \\ 0 & 1 \end{pmatrix} |\psi(0)\rangle, \tag{34}
\]

with

\[
\hat{V}(t_1) = e^{iR_0 t_1} \hat{V} e^{-iR_0 t_1}. \tag{35}
\]

### B. Second order correction

We will find now a similar expression for the second order correction. Expanding again (13) in Taylor series and keeping terms to \( \lambda^2 \), we have

\[
|\psi(t)\rangle \approx \left( \sum_{n=0}^{\infty} \frac{(-it)^n}{n!} \hat{H}_0^n + \lambda \sum_{n=1}^{\infty} \frac{(-it)^n}{n!} \sum_{k=0}^{n-1} \hat{H}_0^{n-1-k} \hat{V} \hat{H}_0^k \right) |\psi(0)\rangle + \lambda^2 \sum_{n=2}^{\infty} \frac{(-it)^n}{n!} \sum_{k=1}^{n-2} \hat{H}_0^{n-2-k-j} \hat{V} \hat{H}_0^j \hat{V} \hat{H}_0^{k-1} |\psi(0)\rangle. \tag{36}
\]

In analogy with the first order correction, we define now the matrix

\[
M = \begin{pmatrix} \hat{H}_0 & \hat{V} & 0 \\ 0 & \hat{H}_0 & \hat{V} \\ 0 & 0 & \hat{H}_0 \end{pmatrix}. \tag{37}
\]

It is very easy to see that in this case

\[
(M^2)_{1,3} = \hat{V}^2, \quad (M^3)_{1,3} = \hat{H}_0 \hat{V}^2 + \hat{V} \hat{H}_0 \hat{V} + \hat{V}^2 \hat{H}_0, \quad \vdots \quad (M^n)_{1,3} = \sum_{k=1}^{n-1} \sum_{j=0}^{n-k} \hat{H}_0^{n-k-j-1} \hat{V} \hat{H}_0^j \hat{V} \hat{H}_0^{k-1};
\]

so we can write equation (36) as

\[
|\psi(t)\rangle \approx e^{-iH_0 t} + \lambda \left( e^{-iM t} \right)_{(1,2)} + \lambda^2 \sum_{n=2}^{\infty} \frac{(-it)^n}{n!} (M^n)_{1,3} |\psi(0)\rangle. \tag{38}
\]
and knowing that
\[(M^0)_{1,3} = (M)_{1,3} = 0,\]
we obtain
\[|\psi(t)| \approx \left( e^{-iH_0t} + \lambda \left( e^{-iM_1} \right)_{1,2} + \lambda^2 \left( e^{-iM_1} \right)_{1,3} \right) |\psi(0)|.\] (39)

Inserting now the matrix
\[||\psi^p|| = \left( \begin{array}{ccc} |\psi(1,1)\rangle & |\psi(1,2)\rangle & |\psi(1,3)\rangle \\
|\psi(2,1)\rangle & |\psi(2,2)\rangle & |\psi(2,3)\rangle \\
|\psi(3,1)\rangle & |\psi(3,2)\rangle & |\psi(3,3)\rangle \end{array} \right),\] (40)
where the first order corrections \(|\psi(1,2)\rangle\) and the second order corrections \(|\psi(1,3)\rangle\) are included. Expanding \(|\psi\rangle\) to second order in \(\lambda\), we get
\[|\psi\rangle \approx |\psi(0)(t)\rangle + \lambda(|\psi^p\rangle)_{1,2} + \lambda^2(|\psi^p\rangle)_{1,3}.\] (41)

Following the same procedure as in the first order correction case, we derive equations (39) and (41) with respect to time, and equate the corresponding equations to obtain
\[i \frac{\partial}{\partial t} |\psi(0)(t)\rangle + i\lambda \frac{\partial}{\partial t} (||\psi^p||)_{1,2} + \lambda^2 \frac{\partial}{\partial t} (||\psi^p||)_{1,3} = \hat{H}_0 e^{-i\hat{H}_0 t} |\psi(0)\rangle + \lambda (Me^{-itM} I |\psi(0)\rangle)_{1,2} + \lambda^2 (Me^{-itM} I |\psi(0)\rangle)_{1,3}.\] (42)

Equating powers of \(\lambda^2\), we can establish that
\[i \frac{\partial}{\partial t} (||\psi^p||)_{1,3} = (Me^{-itM} I |\psi(0)\rangle)_{1,3}.\]

or equivalently
\[i \frac{\partial}{\partial t} ||\psi^p|| = M ||\psi^p||,\] (43)

with the initial condition
\[||\psi^p(0)|| = \left( \begin{array}{ccc} |\psi(0)\rangle & 0 & 0 \\
0 & |\psi(0)\rangle & 0 \\
0 & 0 & |\psi(0)\rangle \end{array} \right).\] (44)

Equation (44) is similar to (24), thus we can again proceed as in the first order case, choosing the third column in both sides of the equation and getting the differential equations system
\[i \frac{\partial}{\partial t} \begin{pmatrix} |\psi(1,3)\rangle \\
|\psi(2,3)\rangle \\
|\psi(3,3)\rangle \end{pmatrix} = M \begin{pmatrix} |\psi(1,3)\rangle \\
|\psi(2,3)\rangle \\
|\psi(3,3)\rangle \end{pmatrix},\] (45)

with the initial condition
\[\begin{pmatrix} 0 \\
0 \\
|\psi(0)\rangle \end{pmatrix}.\] (46)

The correction we were looking for is then
\[|\psi_{1,3}\rangle = -ie^{-iH_0t} \int_0^t e^{iH_0t_1} \hat{V} \left[ -ie^{-iH_0t_1} \int_0^{t_1} e^{iH_0t_2} \hat{V} e^{-iH_0t_2} dt_2 |\psi(0)\rangle \right] dt_1.\] (47)

In this equation we note that the expression inside the square brackets is the first order correction, then using (33) we can write
\[|\psi_{1,3}\rangle = -ie^{-iH_0t} \int_0^t e^{iH_0t_1} \hat{V} \left[ e^{-it_1 E_n^{(0)}} \left( |n(1)\rangle - it_1 |n(0)\rangle \Delta_n^{(1)} - |n(1)\rangle t_1 \right) \right] dt_1.\] (48)
Inserting the identity operator $\hat{I}$ as we had defined it in the first order correction, we have

$$|\psi_{1,3}\rangle = -i \sum_k |k(0)\rangle\langle k(0)| e^{-i\hat{H}_0 t} \int_0^t e^{i\hat{H}_0 t_1} \hat{V} \left[ e^{-it_1 E_n(0)} \left( |n(1)\rangle - it_1 |n(0)\rangle \Delta_n^{(1)} \right) - |n(1)\rangle t_1 \right] dt_1,$$

$$= e^{-iE_n(0)t} \left[ \sum_{k \neq n} \sum_{m \neq n} \left( E_n(0) - E_k(0) \right) \left( E_n(0) - E_m(0) \right) - \sum_{k \neq n} |k(0)\rangle \Delta_n^{(1)} \frac{V_{kn}}{E_n(0) - E_k(0)} - it |n(0)\rangle \hat{V} |n(1)\rangle \right]$$

$$+ it^2 (\Delta_n^{(1)})^2 - \sum_{k \neq n} \frac{it \langle k | (0) \Delta_n^{(1)} V_{kn} (0) | m \rangle}{E_n(0) - E_k(0)} - |n(2)\rangle t + |n(2)\rangle t,$$

with

$$|n^{(2)}(t)| = \sum_{k \neq n} \sum_{m \neq n} \left[ \frac{|k(0)\rangle \langle k(0)|}{(E_n(0) - E_k(0)) (E_n(0) - E_m(0))} - \sum_{k \neq n} \frac{|k(0)\rangle \Delta_n^{(1)} V_{kn} (0) | m \rangle}{(E_n(0) - E_k(0))^2} - \sum_{k \neq n} \frac{it |k(0)\rangle \Delta_n^{(1)} V_{kn} (0) | m \rangle}{E_n(0) - E_k(0)} \right] e^{-iE_n(0)t}$$

and

$$|n^{(2)}(t)| = i \sum_k |k(0)\rangle\langle k(0)| e^{-i\hat{H}_0 t} \int_0^t e^{i\hat{H}_0 t_1} \hat{V} |n(1)\rangle(t_1) dt_1,$$

$$= \sum_{k \neq n} \sum_{m \neq n} \frac{|k(0)\rangle e^{-iE_n(0)t} V_{kn} (0) | m \rangle}{E_n(0) - E_m(0)} \int_0^t e^{i(E_n(0) - E_m(0)) t_1} dt_1$$

In the same way as in the first order correction case, equation (49) gives us the correction to the wave function and to the energy in one operation; however, it generates the additional expressions $|n^{(2)}(t)|$ and $|n^{(2)}(t)|$.

We can show that it may be written in the compact form

$$||\psi^p|| = e^{-it\hat{H}_0} \begin{pmatrix} 1 & -iT_0^1 & \cdots & -iT_{m+1}^1 \\ 0 & 1 & \cdots & -iT_{m+1}^0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & 1 \end{pmatrix} |\psi(0)||,$$  \hspace{1cm} (52)

C. Higher order corrections

In the previous sections, we have found the corrections to first and second order, and we have shown that the results are not only consistent with the traditional perturbation theory, but new terms arise. These new terms will be shown correct in Section IV where we compare both solutions. In rest of this section we generalize our model to higher orders. We propose the perturbation series

$$|\psi^{(0)}(t)| + \sum_{n=1}^m \lambda^n (||\psi^p||)_{1,m+1} \approx \left( e^{-it\hat{H}_0} + \sum_{n=1}^m \lambda^n (e^{-itM}) \right) |\psi(0)|$$  \hspace{1cm} (53)

with

$$||\psi^p|| = \begin{pmatrix} |\psi_{(1,1)}| & \cdots & |\psi_{(1,m+1)}| \\ \vdots & \ddots & \vdots \\ |\psi_{(m+1,1)}| & \cdots & |\psi_{(m+1,m+1)}| \end{pmatrix},$$  \hspace{1cm} (54)

where $m$ is the correction order, and

$$M = \begin{pmatrix} \hat{H}_0 & \hat{V} & \cdots & 0 \\ 0 & \hat{H}_0 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & \cdots & 0 & \hat{H}_0 \end{pmatrix}.$$  \hspace{1cm} (55)
Following the method for the first and second order corrections, we deduce the following system of differential equations

\[ i \frac{\partial}{\partial t} (|\psi^p\rangle)_{1,m+1} = M(|\psi^p\rangle)_{1,m+1}, \] (56)

or

\[ i \frac{\partial}{\partial t} \left( \begin{array}{c} |\psi_{1,m+1}\rangle \\ \vdots \\ |\psi_{m+1,m+1}\rangle \\ \vdots \\ |\psi_{m+1,m+1}\rangle \end{array} \right) = M \left( \begin{array}{c} |\psi_{1,m+1}\rangle \\ \vdots \\ |\psi_{m+1,m+1}\rangle \end{array} \right), \] (57)

with the initial condition

\[ \left( \begin{array}{c} 0 \\ \vdots \\ |\psi(0)\rangle \end{array} \right), \] (58)

so the solution we are looking for is

\[ |\psi_{1,n+1}\rangle = -i e^{-\hat{H}_0 t} \int_0^t e^{i\hat{H}_0 t_1} V \left[ -i e^{-i\hat{H}_0 t_1} \int_0^{t_1} e^{i\hat{H}_0 t_2} V \left[ -i e^{-i\hat{H}_0 t_2} \int_0^{t_2} \cdots dt_3 \right] dt_2 \right] |\psi(0)\rangle \ dt_1. \] (59)

**IV. COMPARISON OF THE STANDARD AND THE MATRIX METHODS**

We will treat now the case of a harmonic oscillator perturbed by a quadratic potential. More than as an example, what we pretend in this section is to show that in this case, where an exact analytic solution is known, our method gives a better solution than the standard Rayleigh-Schrödinger perturbation theory. The non-perturbed Hamiltonian is

\[ \hat{H}_0 = \frac{1}{2} (\hat{p}^2 + \omega^2 \hat{x}^2), \] (60)

and the perturbation potential is

\[ \hat{V} = \frac{\omega^2}{2} \hat{x}^2; \] (61)

for simplicity we consider a unity mass oscillator

The total Hamiltonian is

\[ \hat{H}_\omega = \frac{1}{2} (\hat{p}^2 + \bar{\omega}^2 \hat{x}^2), \] (62)

with

\[ \bar{\omega} = \omega \sqrt{1 + \lambda}. \] (63)

Physically this Hamiltonian can represent a one mode cavity, to which the oscillation frequency can be changed by changing the perturbation parameter. The final result of a modification in the initial frequency produces squeezed coherent states [11], as it is described by Dutra [12].

First we obtain the first order correction with the matrix method we have just introduced. We do so by substituting the perturbation potential in equation (30) and obtain

\[ |\psi_{1,2}\rangle = -i \frac{\omega^2}{2} e^{-i\hat{H}_0 t} \int_0^t e^{i\hat{H}_0 t_1} \hat{x}^2 e^{-i\hat{H}_0 t_1} dt_1 |\psi(0)\rangle. \] (64)

By defining the position operator in terms of annihilation and creation operators, \( \hat{a} \) and \( \hat{a}^\dagger \)

\[ \hat{x} = \frac{\hat{a} + \hat{a}^\dagger}{\sqrt{2\omega}}, \] (65)
we can write equation (64) as
\[ |\psi_{1,2}\rangle = -\frac{i}{4} e^{-iH_0 t} \left[ \int_0^t (\hat{a}^2 e^{-2i\omega t} + \hat{a}\hat{a}' + \hat{a}'\hat{a} + (\hat{a}')^2 e^{2i\omega t}) dt \right] |\psi(0)\rangle. \] (66)

Using the relations
\[ e^{iH_0 t} \hat{a} e^{-iH_0 t} = \hat{a} e^{-i\omega t}, \] (67)
and
\[ e^{iH_0 t} \hat{a}' e^{-iH_0 t} = \hat{a}' e^{i\omega t}, \] (68)
equation (66) is transformed in
\[ |\psi_{1,2}\rangle = -\frac{i}{4} e^{-iH_0 t} \left[ \int_0^t (\hat{a}^2 e^{-2i\omega t} + \hat{a}\hat{a}' + \hat{a}'\hat{a} + (\hat{a}')^2 e^{2i\omega t}) dt \right] |\psi(0)\rangle, \]
\[ = -\frac{i}{4} e^{-iH_0 t} \left[ \frac{\hat{a}^2}{-2i\omega} (e^{-2i\omega t} - 1) + \frac{(\hat{a})^2}{2i\omega} (e^{2i\omega t} - 1) + t(\hat{a}\hat{a}' + \hat{a}'\hat{a}) \right] |\psi(0)\rangle. \] (69)

By writing the unperturbed Hamiltonian in terms of the number operator \( \hat{n} = \hat{a}^\dagger \hat{a} \) and using \( |\psi(0)\rangle = |n^{(0)}\rangle = \) we obtain
\[ |\psi_{1,2}\rangle = e^{-iE_n^{(0)} t} \left[ \left( \frac{\sqrt{n(n-1)}}{8} |n^{(0)} - 2^{(0)}\rangle - \frac{\sqrt{(n+1)(n+2)}}{8} |n^{(0)} + 2^{(0)}\rangle \right) - |n^{(0)}\rangle \frac{i\omega}{4}(2n + 1)t \right] \]
\[ - \left( e^{-iE_{n+1}^{(0)} t} \frac{\sqrt{n(n-1)}}{8} |n^{(0)} - 2^{(0)}\rangle - e^{-iE_{n-1}^{(0)} t} \frac{\sqrt{(n+1)(n+2)}}{8} |n^{(0)} + 2^{(0)}\rangle \right). \] (70)

Comparing with (63), we have that
\[ |n^{(1)}\rangle = \frac{\sqrt{n(n-1)}}{8} |n^{(0)} - 2^{(0)}\rangle - \frac{\sqrt{(n+1)(n+2)}}{8} |n^{(0)} + 2^{(0)}\rangle, \] (71)
\[ \Delta_n^{(1)} = \frac{\omega}{4} (2n + 1), \] (72)
and
\[ |n^{(1)}\rangle_t = e^{-iE_{n-1}^{(0)} t} \frac{\sqrt{n(n-1)}}{8} |n^{(0)} - 2^{(0)}\rangle - e^{-iE_{n+1}^{(0)} t} \frac{\sqrt{(n+1)(n+2)}}{8} |n^{(0)} + 2^{(0)}\rangle, \] (73)
with \( E_n^{(0)} = \omega(n + 1/2). \)

As we can see (71) and (72) are the corresponding expressions to the corrections to the wave function and to the energy to first order that are obtained when the stationary Schrödinger equation is considered, while (63) is similar to (71), but with the difference that this expression has time dependent factors.

A. Exact solution

We may see already differences between both methods. In order to compare them, we need to use an example that may be solved, such that, once we have the exact solution, this can be expanded on a (perturbation) parameter and see if it matches the results we obtained.

In this case, the exact formal solution is given by
\[ |\psi(t)\rangle = e^{-iH_o t} |\psi(0)\rangle. \] (74)
where $\hat{H}_\omega$ is the complete Hamiltonian defined in [62].

As usual, we introduce the ladder operators

$$\hat{A}^\dagger = \sqrt{\frac{\omega}{2}} \hat{x} - i \frac{\hat{p}}{\sqrt{2\omega}}$$

(75)

and

$$\hat{A} = \sqrt{\frac{\omega}{2}} \hat{x} + i \frac{\hat{p}}{\sqrt{2\omega}}.$$  

(76)

in terms of which the perturbed Hamiltonian (62) can be written as

$$\hat{H}_\omega = \omega \left( \hat{A}^\dagger \hat{A} + \frac{1}{2} \right).$$  

(77)

It is easy to show that

$$\hat{A}^\dagger = \sqrt{\frac{\omega}{2}} \hat{a} + \hat{a}^\dagger \sqrt{\frac{\omega}{2}} - \sqrt{\frac{\omega}{2}} (\hat{a} - \hat{a}^\dagger)$$

(78)

and

$$\hat{A} = \sqrt{\frac{\omega}{2}} \hat{a} + \hat{a}^\dagger \sqrt{\frac{\omega}{2}} + \sqrt{\frac{\omega}{2}} (\hat{a} - \hat{a}^\dagger).$$

(79)

Defining the squeeze operator [11]

$$\hat{S}(\lambda) = \exp \left\{ \frac{\ln(1 + \lambda)}{8} [\hat{a}^2 - (\hat{a}^\dagger)^2] \right\},$$

(80)

it can be shown that

$$\hat{A} = \hat{S} \hat{a} \hat{S}^\dagger$$

(81)

and

$$\hat{A}^\dagger = \hat{S} \hat{a}^\dagger \hat{S}^\dagger.$$  

(82)

Thus, the formal solution (74) can be written as

$$|\psi(t)\rangle = e^{-i\omega (\hat{A}^\dagger \hat{A} + 1/2)} |\psi(0)\rangle,$$

$$= e^{-i\omega \hat{S}(\hat{a}^\dagger \hat{a} + 1/2) \hat{S}^\dagger} |\psi(0)\rangle,$$

$$= \hat{S} e^{-it\omega (\hat{a}^\dagger \hat{a} + 1/2)} \hat{S}^\dagger |\psi(0)\rangle,$$

and multiplying by $e^{-it\omega (\hat{a}^\dagger \hat{a} + 1/2)} e^{it\omega (\hat{a} \hat{a} + 1/2)}$, we get

$$|\psi(t)\rangle = e^{-it\omega (\hat{a}^\dagger \hat{a} + 1/2)} e^{it\omega (\hat{a} \hat{a} + 1/2)} \hat{S} e^{-it\omega (\hat{a}^\dagger \hat{a} + 1/2)} \hat{S}^\dagger |\psi(0)\rangle.$$  

(83)

We define now the time dependent squeezing operator

$$\hat{S}_\omega (\lambda, t) = e^{it\omega (\hat{a} \hat{a} + 1/2)} \hat{S} e^{-it\omega (\hat{a}^\dagger \hat{a} + 1/2)},$$

$$= e^{it\omega (\hat{a} \hat{a} + 1/2)} e^{\frac{i}{8} \ln(1 + \lambda)} (\hat{a}^2 - (\hat{a}^\dagger)^2) e^{-it\omega (\hat{a}^\dagger \hat{a} + 1/2)},$$

$$= \exp \left\{ \frac{1}{8} \ln(1 + \lambda) \left( e^{it\omega (\hat{a} \hat{a} + 1/2)} \hat{a}^2 e^{-it\omega (\hat{a}^\dagger \hat{a} + 1/2)} - e^{it\omega (\hat{a} \hat{a} + 1/2)} \hat{a} \hat{a}^\dagger e^{-it\omega (\hat{a}^\dagger \hat{a} + 1/2)} \right) \right\},$$

$$= e^{it\omega (\hat{a} \hat{a} + 1/2)} (\hat{a} \hat{a}^\dagger)^2 e^{-it\omega (\hat{a}^\dagger \hat{a} + 1/2)}.$$
and we have
\[ \hat{S}_\omega(\lambda, t) = \exp \left\{ \frac{\ln(1 + \lambda)}{8} [e^{-2it\hat{\omega}} \hat{a}^2 - e^{2it\hat{\omega}} (\hat{a}^\dagger)^2 - \hat{a}^2 e^{-2it\hat{\omega}} - \hat{a}^\dagger e^{2it\hat{\omega}}] \right\}, \] (84)

taking (84) the final form
\[ |\psi(t)\rangle = e^{-it\hat{\omega} t} \hat{S}_\omega(\lambda, t) \hat{S}_\omega^\dagger(\lambda)|\psi(0)\rangle. \] (85)

Up to now we have an exact result. In order to compare with the approximation found with our method, we expand the operators in the above expression in Taylor series in terms of the "small" parameter \( \lambda \). First, we have to first order in \( \lambda \),
\[ e^{-it\hat{\omega} t} \hat{a}^\dagger \hat{a} + \frac{1}{2} \approx 1 + (-it) \frac{\lambda}{2} \hat{H}_0. \] (86)

Second, we write
\[ \hat{S}_\omega^\dagger(\lambda) = \sum_{n=0}^{\infty} \frac{\hat{S}_\omega^{(n)}(0)}{n!} \lambda^n; \] (87)
we keep first order terms, so
\[ \hat{S}_\omega^\dagger(\lambda) \approx \hat{S}_\omega^\dagger(0) + \lambda \hat{S}_\omega^\dagger(1)(0) \] (88)
and because
\[ \hat{S}_\omega^\dagger(0) = 1, \] (89)
and
\[ \hat{S}_\omega^\dagger(1)(0) = \left[ \frac{\partial \hat{S}_\omega^\dagger(\lambda)}{\partial \lambda} \right]_{\lambda=0} = \frac{((\hat{a}^\dagger)^2 - \hat{a}^2)}{8}, \] (90)
so to first order in \( \lambda \)
\[ \hat{S}_\omega^\dagger(\lambda) \approx 1 + \lambda \frac{((\hat{a}^\dagger)^2 - \hat{a}^2)}{8}. \] (91)

Third, we write
\[ \hat{S}_\omega(\lambda, t) = \sum_{n=0}^{\infty} \frac{\hat{S}_\omega^{(n)}(0)}{n!} \lambda^n \] (92)
and it can be shown, that
\[ \hat{S}_\omega^{(0)}(0) = 1 \] (93)
and that
\[ \hat{S}_\omega^{(1)}(0) = \left[ \frac{\partial \hat{S}_\omega(\lambda)}{\partial \lambda} \right]_{\lambda=0} = \frac{1}{8}[\hat{a}^2 e^{-2it\omega} - (\hat{a}^\dagger)^2 e^{2it\omega}], \] (94)
so to first order in \( \lambda \)
\[ \hat{S}_\omega(\lambda, t) \approx 1 + \frac{\lambda}{8}[\hat{a}^2 e^{-2it\omega} - (\hat{a}^\dagger)^2 e^{2it\omega}]. \] (95)

Finally, we arrive to the expression to order one in \( \lambda \)
\[ |\psi(t)\rangle \approx e^{-it\hat{H}_0} \left( 1 + \frac{\lambda}{8} \left( (\hat{a}^\dagger)^2 (1 - e^{2it\omega}) + \hat{a}^2 (e^{-2it\omega} - 1) \right) - \frac{it\omega}{2} \left( \hat{n} + \frac{1}{2} \right) \right) |\psi(0)\rangle, \] (96)
that when \(|n^{(0)}\rangle\) is taken as initial condition, formula (69) is recovered, that is the one obtained from the method introduced here.

The development to second order is long and bothersome and we do not present it here, but we recover the expressions found with our method in the previous section.
V. THE DYSON SERIES IN THE MATRIX METHOD

It is well known that in terms of the Dyson series \(13\), the wavefunctions of the perturbed problem are written as

\[
|\psi(t)\rangle = e^{-i\hat{H}_0 t} \hat{T} \left\{ \exp \left[ -i\lambda \int_0^t dt_1 \hat{V}(t_1) \right] \right\} |\psi(0)\rangle. \tag{97}
\]

where \(\hat{T}\) is the time order operator \(14\); i.e., if we have the time dependent operators \(\hat{A}(t)\) and \(\hat{B}(t)\) then

\[
\hat{T}[\hat{A}(t_1)\hat{B}(t_2)] = \begin{cases} 
\hat{B}(t_2)\hat{A}(t_1) & \text{if } t_2 > t_1, \\
\hat{A}(t_1)\hat{B}(t_2) & \text{if } t_1 > t_2.
\end{cases} \tag{98}
\]

On the other hand, from equation (53) we can write

\[
|\psi(t)\rangle = \left( e^{-i\hat{H}_0 t} + \sum_{n=1}^{\infty} \lambda^n \left( e^{-i\hat{M}t} \right)_{(1,n+1)} \right) |\psi(0)\rangle; \tag{99}
\]

so comparing equation (97) with equation (99), we derive the formula

\[
\hat{T} \left\{ \exp \left[ -i\lambda \int_0^t dt_1 \hat{V}(t_1) \right] \right\} = e^{i\hat{H}_0 t} \sum_{n=0}^{\infty} \lambda^n \left( e^{-i\hat{M}t} \right)_{(1,n+1)}.
\]

which offers a matrix expansion for the Dyson operator and that links our matrix method with the Dyson series.

VI. CONCLUSIONS

In this work, we have developed a new technique to find approximate solutions to the Schrödinger equation. We used the formal solution of the time dependent Schrödinger equation \(12\). The key ingredient is the introduction of the matrix \(M\) defined in \(53\) that allows us the transformation of the Taylor series for the wave function, in terms of products of the operators \(\hat{H}_0\) and \(\hat{V}\), in a series of powers of the matrix \(M\), that is easier to handle.

The method allowed us to express the terms of the perturbation series in the form of integrals that depend on time that are restricted to the interval \([0,t]\), as appears in \(30\) and \(47\). An interesting property of these equations is that in the form that are presented they do not distinguish if the Hamiltonian \(\hat{H}_0\) is degenerate or not, for what the equations that we provide for the corrections are very general expressions.

To test our method versus the standard Rayleigh-Schrödinger theory, we solved the corrections to the first and second order of quadratic potential as perturbation on the harmonic oscillator, and we found that the solution not only contains the results of the stationary case, but we find other time dependent terms that help us to study the temporal evolution of the corrections. It is important to remark that the terms as \(32\), \(50\), \(51\) among others could not be found in the conventional treatment of the perturbation theory.

Finally, we have given an alternative expression for the Dyson series in a matrix form.

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