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Alternative analysis to perturbation theory in quantum mechanics

Dyson series in matrix form

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Abstract. We develop an alternative approach to the 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 for any initial condition, which may be bothersome in the standard method. 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.

1 Introduction

The Schrödinger equation [1] 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 [2,3] and the Morse potential [4]. 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 [5] for instance. When an exact analytical solution can not be found, we are forced to apply approximation methods [3,6], 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 [7] 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 [8] to those more mathematical and fundamental, as convergency problems [9,10]. The Rayleigh-Schrödinger theory is appropriate when we have a time independent Hamiltonian, that can be separated in two parts, as follows:

$$\hat{H} = \hat{H}_0 + \hat{H}_{\mathrm{p}}, \tag{1}$$

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

$$\hat{H}_0|n^{(0)}\rangle = E_n^{(0)}|n^{(0)}\rangle \tag{2}$$

are known. The second part of the Hamiltonian, $\hat{H}_{\mathrm{p}}$, is *small* compared to H_0; thus $\hat{H}_{\mathrm{p}}$ 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 $\hat{H}_{\mathrm{p}}$ in terms of a dimensionless real parameter λ, which is considered very small compared to one

$$\hat{H}_{\mathrm{p}} = \lambda \hat{V} \qquad (\lambda \ll 1). \tag{3}$$

Here, we propose an alternative perturbation method based on the evolution operator for Hamiltonian (1), 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 2, 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 3, 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

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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 4 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, λ. In Section 5 we apply our formalism to rewrite the Dyson series in matrix form and Section 6 is left for conclusions.

2 Standard 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

$$E_n = E_n^{(0)} + \lambda \Delta_n^{(1)} + \lambda^2 \Delta_n^{(2)} + \cdots , \tag{4}$$

and the eigenfunctions

$$|n\rangle = |n^{(0)}\rangle + \lambda |n^{(1)}\rangle + \lambda^2 |n^{(2)}\rangle + \cdots \tag{5}$$

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

$$\Delta_n^{(1)} = \langle n^{(0)}|\hat{V}|n^{(0)}\rangle = V_{nn} \tag{6}$$

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

where we have defined

$$V_{kn} = \langle k^{(0)}|\hat{V}|n^{(0)}\rangle. \tag{8}$$

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

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

and

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

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.

3 Matrix approach to the perturbation theory

3.1 First order correction

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

$$i\frac{\partial}{\partial t}|\psi\rangle = \hat{H}|\psi\rangle = \left(\hat{H}_0 + \lambda\hat{V}\right)|\psi\rangle. \tag{11}$$

The formal solution may be written as

$$|\psi(t)\rangle = e^{-it(\hat{H}_0+\lambda\hat{V})}|\psi(0)\rangle, \tag{12}$$

that by expanding the exponential in a Taylor series

$$|\psi(t)\rangle = \sum_{n=0}^{\infty} \frac{(-it)^n}{n!}\left(\hat{H}_0 + \lambda\hat{V}\right)^n |\psi(0)\rangle, \tag{13}$$

is obtained. If we develop the binomials inside the summation, rearrange terms and cut the series to first order in λ, we have

$$|\psi(t)\rangle \approx \sum_{n=0}^{\infty} \frac{(-it)^n}{n!}\hat{H}_0^n|\psi(0)\rangle + \lambda \sum_{n=1}^{\infty} \frac{(-it)^n}{n!} \sum_{k=0}^{n-1} \hat{H}_0^{n-1-k}\hat{V}\hat{H}_0^k \times |\psi(0)\rangle. \tag{14}$$

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

$$\begin{aligned} (M)_{1,2} &= \hat{V}, \\ (M^2)_{1,2} &= \hat{H}_0\hat{V} + \hat{V}\hat{H}_0, \\ &\vdots \\ (M^n)_{1,2} &= \sum_{k=0}^{n-1} \hat{H}_0^{n-1-k}\hat{V}\hat{H}_0^k. \end{aligned}$$

Thus, equation (14) can be written as

$$|\psi(t)\rangle \approx \left[\sum_{n=0}^{\infty} \frac{(-it)^n}{n!}(\hat{H}_0)^n + \lambda \sum_{n=1}^{\infty} \frac{(-it)^n (M^n)_{(1,2)}}{n!}\right]|\psi(0)\rangle. \tag{16}$$

As $M^0 = I$ (where I is the $[2\times 2]$ identity matrix), we trivially have that $(M^0)_{(1,2)} = 0$. By substituting this term in equation (16) we obtain

$$\begin{aligned} |\psi(t)\rangle &\approx \left(e^{-i\hat{H}_0 t} + \lambda\left(e^{-iMt}\right)_{(1,2)}\right)|\psi(0)\rangle \\ &= e^{-i\hat{H}_0 t}|\psi(0)\rangle + \lambda\left(e^{-iMt}\right)_{(1,2)}|\psi(0)\rangle. \end{aligned} \tag{17}$$

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

$$|\psi(t)\rangle \approx |\psi^{(0)}(t)\rangle + \lambda(||\psi^p\rangle)_{1,2}, \tag{18}$$

where we have defined the *matrix wave function*

$$||\psi^p\rangle = \begin{pmatrix} |\psi_{(1,1)}\rangle & |\psi_{(1,2)}\rangle \\ |\psi_{(2,1)}\rangle & |\psi_{(2,2)}\rangle \end{pmatrix}. \tag{19}$$

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

$$i\frac{\partial}{\partial t}|\psi^{(0)}(t)\rangle + i\lambda\frac{\partial}{\partial t}(||\psi^p\rangle)_{1,2} = \hat{H}_0 e^{-i\hat{H}_0 t}|\psi(0)\rangle + \lambda\left(Me^{-itM}I|\psi(0)\rangle\right)_{1,2}. \tag{20}$$

Equating powers of λ, we have

$$i\frac{\partial}{\partial t}(\|\psi^p\rangle)_{1,2} = \left(Me^{-itM}I|\psi(0)\rangle\right)_{1,2}. \tag{21}$$

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

$$i\frac{\partial}{\partial t}\begin{pmatrix} |\psi_{(1,1)}\rangle & |\psi_{(1,2)}\rangle \\ |\psi_{(2,1)}\rangle & |\psi_{(2,2)}\rangle \end{pmatrix} = Me^{-itM}\begin{pmatrix} |\psi(0)\rangle & 0 \\ 0 & |\psi(0)\rangle \end{pmatrix}. \tag{22}$$

Integrating this equation, we have

$$||\psi^p\rangle = e^{-itM}\begin{pmatrix} |\psi(0)\rangle & 0 \\ 0 & |\psi(0)\rangle \end{pmatrix}, \tag{23}$$

to finally write the differential equation

$$i\frac{\partial}{\partial t}||\psi^p\rangle = M||\psi^p\rangle, \tag{24}$$

with the initial condition

$$||\psi^p(0)\rangle = \begin{pmatrix} |\psi(0)\rangle & 0 \\ 0 & |\psi(0)\rangle \end{pmatrix}. \tag{25}$$

The needed solution is associated with the second column of matrix $||\psi^p\rangle$, thus we write

$$i\frac{\partial}{\partial t}\begin{pmatrix} |\psi_{(1,2)}\rangle \\ |\psi_{(2,2)}\rangle \end{pmatrix} = M\begin{pmatrix} |\psi_{(1,2)}\rangle \\ |\psi_{(2,2)}\rangle \end{pmatrix}, \tag{26}$$

but because M is a tridiagonal matrix, the system may be directly integrated. We show it by writing explicitly

$$i\frac{\partial}{\partial t}|\psi_{(1,2)}\rangle = \hat{H}_0|\psi_{(1,2)}\rangle + \hat{V}|\psi_{(2,2)}\rangle, \tag{27}$$

and

$$i\frac{\partial}{\partial t}|\psi_{(2,2)}\rangle = \hat{H}_0|\psi_{(2,2)}\rangle, \tag{28}$$

with the initial condition

$$\begin{pmatrix} 0 \\ |\psi(0)\rangle \end{pmatrix}. \tag{29}$$

Because we know the solution for $\hat{H}_0$, equation (28) is solved trivially,

$$|\psi_{(2,2)}\rangle = e^{-it\hat{H}_0}|\psi(0)\rangle, \tag{30}$$

that substituted in (27), allows us to write

$$i\frac{\partial}{\partial t}|\psi_{(1,2)}\rangle = \hat{H}_0|\psi_{(1,2)}\rangle + \hat{V}e^{-i\hat{H}_0 t}|\psi(0)\rangle. \tag{31}$$

Making the transformation $|\psi_{(1,2)}\rangle = e^{-i\hat{H}_0}|\phi_{1,2}(x)\rangle$, we arrive to the equation

$$i\frac{\partial}{\partial t}|\phi_{1,2}\rangle = e^{i\hat{H}_0 t}\hat{V}e^{-i\hat{H}_0 t}|\psi(0)\rangle, \tag{32}$$

that can be easily integrated to give

$$|\phi_{1,2}\rangle = -i\int_0^t e^{i\hat{H}_0 t_1}\hat{V}e^{-i\hat{H}_0 t_1}dt_1|\psi(0)\rangle, \tag{33}$$

and by transforming back the solution to the first correction may be obtained

$$|\psi_{1,2}\rangle = -ie^{-i\hat{H}_0 t}\int_0^t e^{i\hat{H}_0 t_1}\hat{V}e^{-i\hat{H}_0 t_1}dt_1|\psi(0)\rangle. \tag{34}$$

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.

Additionally we can show that we can write

$$||\psi^p\rangle = e^{-it\hat{H}_0}\begin{pmatrix} 1 & -i\int_0^t dt_1\hat{V}(t_1) \\ 0 & 1 \end{pmatrix}|\psi(0)\rangle, \tag{35}$$

with

$$\hat{V}(t_1) = e^{i\hat{H}_0 t_1}\hat{V}e^{-i\hat{H}_0 t_1}. \tag{36}$$

3.2 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 λ^2, we have

$$|\psi(t)\rangle \approx \sum_{n=0}^{\infty}\frac{(-it)^n}{n!}\hat{H}_0^n|\psi(0)\rangle + \lambda\sum_{n=1}^{\infty}\frac{(-it)^n}{n!}\sum_{k=0}^{n-1}\hat{H}_0^{n-1-k}\hat{V}\hat{H}_0^k|\psi(0)\rangle + \lambda^2\sum_{n=2}^{\infty}\frac{(-it)^n}{n!}\sum_{k=1}^{n-1}\sum_{j=0}^{n-k}\hat{H}_0^{n-k-j-1}\hat{V}\hat{H}_0^j\hat{V}\hat{H}_0^{k-1}|\psi(0)\rangle. \tag{37}$$

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

$$M = \begin{pmatrix} \hat{H}_0 & \hat{V} & 0 \\ 0 & \hat{H}_0 & \hat{V} \\ 0 & 0 & \hat{H}_0 \end{pmatrix}. \tag{38}$$

It is very easy to see that in this case

$$(M^2)_{1,3} = \hat{V}^2, \tag{39}$$

$$(M^3)_{1,3} = \hat{H}_0\hat{V}^2 + \hat{V}\hat{H}_0\hat{V} + \hat{V}^2\hat{H}_0, \tag{40}$$

$$\vdots \tag{41}$$

$$(M^n)_{1,3} = \sum_{k=1}^{n-1}\sum_{j=0}^{n-k} \hat{H}_0^{n-k-j-1}\hat{V}\hat{H}_0^j\hat{V}(\hat{H}_0)^{k-1}; \tag{42}$$

so we can write equation (37) as

$$|\psi(t)\rangle \approx [e^{-i\hat{H}_0 t} + \lambda\left(e^{-iMt}\right)_{(1,2)} + \lambda^2\sum_{n=2}^{\infty}\frac{(-it)^n}{n!}(M^n)_{1,3}]|\psi(0)\rangle, \tag{43}$$

and using that $\left(M^0\right)_{1,3} = (M)_{1,3} = 0$, we obtain

$$|\psi(t)\rangle \approx (e^{-i\hat{H}_0 t} + \lambda\left(e^{-iMt}\right)_{(1,2)} + \lambda^2\left(e^{-iMt}\right)_{(1,3)})|\psi(0)\rangle. \tag{44}$$

Inserting now the matrix

$$||\psi^p\rangle = \begin{pmatrix} |\psi_{(1,1)}\rangle & |\psi_{(1,2)}\rangle & |\psi_{(1,3)}\rangle \\ |\psi_{(2,1)}\rangle & |\psi_{(2,2)}\rangle & |\psi_{(2,3)}\rangle \\ |\psi_{(3,1)}\rangle & |\psi_{(3,2)}\rangle & |\psi_{(3,3)}\rangle \end{pmatrix}, \tag{45}$$

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 λ, we get

$$|\psi\rangle \approx |\psi^{(0)}(t)\rangle + \lambda(||\psi^p\rangle)_{1,2} + \lambda^2(||\psi^p\rangle)_{1,3}. \tag{46}$$

Following the same procedure as in the first order correction case, we derive equations (44) and (46) with respect to time, and equate the corresponding equations to obtain

$$i\frac{\partial}{\partial t}|\psi^{(0)}(t)\rangle + i\lambda\frac{\partial}{\partial t}(||\psi^p\rangle)_{1,2} + \lambda^2\frac{\partial}{\partial t}(||\psi^p\rangle)_{1,3} = \hat{H}_0 e^{-i\hat{H}_0 t}|\psi(0)\rangle + \lambda\left(Me^{-itM}I|\psi(0)\rangle\right)_{1,2} + \lambda^2\left(Me^{-itM}I|\psi(0)\rangle\right)_{1,3}. \tag{47}$$

Equating powers of λ^2, we can establish that

$$i\frac{\partial}{\partial t}(||\psi^p\rangle)_{1,3} = \left(Me^{-itM}I|\psi(0)\rangle\right)_{1,3}. \tag{48}$$

or equivalently

$$i\frac{\partial}{\partial t}||\psi^p\rangle = M||\psi^p\rangle, \tag{49}$$

with the initial condition

$$||\psi^p(0)\rangle = \begin{pmatrix} |\psi(0)\rangle & 0 & 0 \\ 0 & |\psi(0)\rangle & 0 \\ 0 & 0 & |\psi(0)\rangle \end{pmatrix}. \tag{50}$$

Equation (50) 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

$$i\frac{\partial}{\partial t}\begin{pmatrix} |\psi_{(1,3)}\rangle \\ |\psi_{(2,3)}\rangle \\ |\psi_{(3,3)}\rangle \end{pmatrix} = M\begin{pmatrix} |\psi_{(1,3)}\rangle \\ |\psi_{(2,3)}\rangle \\ |\psi_{(3,3)}\rangle \end{pmatrix}, \tag{51}$$

with the initial condition

$$\begin{pmatrix} 0 \\ 0 \\ |\psi(0)\rangle \end{pmatrix}. \tag{52}$$

The correction we were looking for is then

$$|\psi_{1,3}\rangle = (-i)^2 e^{-i\hat{H}_0 t}\int_0^t\int_0^{t_1} e^{i\hat{H}_0 t_1}\hat{V}e^{-i\hat{H}_0 t_1} \times e^{i\hat{H}_0 t_2}\hat{V}e^{-i\hat{H}_0 t_2}dt_2 dt_1|\psi(0)\rangle. \tag{53}$$

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

$$||\psi^p\rangle = e^{-it\hat{H}_0} \times \begin{pmatrix} 1 & -i\int_0^t dt_1\hat{V}(t_1) & (-i)^2\int_0^t dt_1\int_0^{t_1}dt_2\hat{V}(t_1)\hat{V}(t_2) \\ 0 & 1 & -i\int_0^t dt_1\hat{V}(t_1) \\ 0 & 0 & 1 \end{pmatrix} \times |\psi(0)\rangle. \tag{54}$$

3.3 Higher order corrections

In this subsection we generalize our method to higher orders. We propose the perturbation series

$$|\psi^{(0)}(t)\rangle + \sum_{n=1}^{m}\lambda^n(||\psi^p\rangle)_{1,m+1} \approx \left(e^{-it\hat{H}_0} + \sum_{n=1}^{m}\lambda^n\left(e^{-itM}\right)\right)|\psi(0)\rangle \tag{55}$$

with

$$||\psi^p\rangle = \begin{pmatrix} |\psi_{(1,1)}\rangle & \cdots & |\psi_{(1,m+1)}\rangle \\ \vdots & \ddots & \vdots \\ |\psi_{(m+1,1)}\rangle & \cdots & |\psi_{(m+1,m+1)}\rangle \end{pmatrix}, \tag{56}$$

where m is the correction order, and

$$M = \begin{pmatrix} \hat{H}_0 & \hat{V} & \cdots & 0 \\ 0 & \hat{H}_0 & \cdots & 0 \\ \vdots & & \ddots & \vdots \\ 0 & \cdots & & \hat{H}_0 \end{pmatrix}. \tag{57}$$

Following the method for the first and second order corrections, we deduce the following system of differential equations

$$i\frac{\partial}{\partial t}(||\psi^p\rangle)_{1,m+1} = M(||\psi^p\rangle)_{1,m+1}, \tag{58}$$

or

$$i\frac{\partial}{\partial t}\begin{pmatrix}|\psi_{1,m+1}\rangle\\ \vdots\\ |\psi_{m+1,m+1}\rangle\end{pmatrix}=M\begin{pmatrix}|\psi_{1,m+1}\rangle\\ \vdots\\ |\psi_{m+1,m+1}\rangle\end{pmatrix},\tag{59}$$

with the initial condition

$$\begin{pmatrix}0\\ \vdots\\ |\psi(0)\rangle\end{pmatrix},\tag{60}$$

so the solution we are looking for is

$$|\psi_{1,n+1}\rangle=(-i)^n e^{-iH_0t}\int_0^t\int_0^{t_1}\int_0^{t_2}e^{iH_0t_1}Ve^{-iH_0t_1}\times e^{iH_0t_2}Ve^{-iH_0t_2}\cdots dt_3dt_2dt_1|\psi(0)\rangle.\tag{61}$$

4 Quadratic potential as an example

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 if the known analytic solution is expanded, it gives the one obtained with our method. The non-perturbed Hamiltonian is

$$\hat{H}_0=\frac{1}{2}(\hat{p}^2+\omega^2\hat{x}^2),\tag{62}$$

and the perturbation potential is

$$\hat{V}=\frac{\omega^2}{2}\hat{x}^2;\tag{63}$$

for simplicity we consider a unity mass oscillator.
The total Hamiltonian is

$$\hat{H}_{\tilde{\omega}}=\frac{1}{2}(\hat{p}^2+\tilde{\omega}^2\hat{x}^2),\tag{64}$$

with

$$\tilde{\omega}=\omega\sqrt{1+\lambda}.\tag{65}$$

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 (34) and obtain

$$|\psi_{1,2}\rangle=-i\frac{\omega^2}{2}e^{-i\hat{H}_0t}\int_0^t e^{i\hat{H}_0t_1}\hat{x}^2e^{-i\hat{H}_0t_1}dt_1|\psi(0)\rangle.\tag{66}$$

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

$$\hat{x}=\frac{\hat{a}+\hat{a}^\dagger}{\sqrt{2\omega}},\tag{67}$$

we can write equation (66) as

$$|\psi_{1,2}\rangle=-i\frac{\omega}{4}e^{-i\hat{H}_0t}\int_0^t e^{i\hat{H}_0t_1}\left(\hat{a}+\hat{a}^\dagger\right)^2e^{-i\hat{H}_0t_1}dt_1|\psi(0)\rangle.\tag{68}$$

By using the relations $e^{i\hat{H}_0t}\hat{a}e^{-i\hat{H}_0t}=\hat{a}e^{-i\omega t}$, $e^{i\hat{H}_0t}\hat{a}^\dagger e^{-i\hat{H}_0t}=\hat{a}^\dagger e^{i\omega t}$ equation (68) is transformed in

$$|\psi_{1,2}\rangle=-i\frac{\omega}{4}e^{-i\hat{H}_0t}[\frac{\hat{a}^2}{-2i\omega}\left(e^{-2i\omega t}-1\right)+\frac{(\hat{a}^\dagger)^2}{2i\omega}\left(e^{2i\omega t}-1\right)+t(\hat{a}\hat{a}^\dagger+\hat{a}^\dagger\hat{a})]|\psi(0)\rangle.\tag{69}$$

4.1 Exact solution

In order to check that our method gives good results we now give the exact solution of this problem, to later do an expansion and be able to compare with the solution given above.

In this case, the exact formal solution is given by

$$|\psi(t)\rangle=e^{-i\hat{H}_{\tilde{\omega}}t}|\psi(0)\rangle.\tag{70}$$

where $\hat{H}_{\tilde{\omega}}$ is the complete Hamiltonian defined in (64). As usual, we introduce the ladder operators

$$\hat{A}^\dagger=\sqrt{\frac{\tilde{\omega}}{2}}\hat{x}-i\frac{\hat{p}}{\sqrt{2\tilde{\omega}}}\tag{71}$$

and

$$\hat{A}=\sqrt{\frac{\tilde{\omega}}{2}}\hat{x}+i\frac{\hat{p}}{\sqrt{2\tilde{\omega}}}.\tag{72}$$

in terms of which the perturbed Hamiltonian (64) can be written as

$$\hat{H}_{\tilde{\omega}}=\tilde{\omega}\left(\hat{A}^\dagger\hat{A}+\frac{1}{2}\right).\tag{73}$$

It is easy to show that

$$\hat{A}^\dagger=\sqrt{\frac{\tilde{\omega}}{2}}\frac{\hat{a}+\hat{a}^\dagger}{\sqrt{2\omega}}-\sqrt{\frac{\omega}{2}}\frac{(\hat{a}-\hat{a}^\dagger)}{\sqrt{2\tilde{\omega}}}\tag{74}$$

and

$$\hat{A}=\sqrt{\frac{\tilde{\omega}}{2}}\frac{\hat{a}+\hat{a}^\dagger}{\sqrt{2\omega}}+\sqrt{\frac{\omega}{2}}\frac{(\hat{a}-\hat{a}^\dagger)}{\sqrt{2\tilde{\omega}}}.\tag{75}$$

Defining the squeeze operator [11]

$$\hat{S}(\lambda)=\exp\left\{\frac{\ln(1+\lambda)}{8}\left[\hat{a}^2-(\hat{a}^\dagger)^2\right]\right\},\tag{76}$$

it can be shown that

$$\hat{A}=\hat{S}\hat{a}\hat{S}^\dagger,\qquad \hat{A}^\dagger=\hat{S}\hat{a}^\dagger\hat{S}^\dagger.\tag{77}$$

Thus, the formal solution (70) can be written as

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

or

$$|\psi(t)\rangle = e^{-it\tilde{\omega}(\hat{a}^\dagger\hat{a}+1/2)}\hat{S}_{\tilde{\omega}}(\lambda,t)\hat{S}^\dagger(\lambda)|\psi(0)\rangle, \tag{78}$$

with

$$\hat{S}_{\tilde{\omega}}(\lambda,t) = \exp\left\{\frac{\ln(1+\lambda)}{8}\left[e^{-2it\tilde{\omega}}\hat{a}^2 - e^{2it\tilde{\omega}}(\hat{a}^\dagger)^2\right]\right\}. \tag{79}$$

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 λ. First, we have to first order in λ,

$$e^{-it\tilde{\omega}(\hat{a}^\dagger\hat{a}+1/2)} = e^{-it\frac{\tilde{\omega}}{\omega}\hat{H}_0} \approx 1 + (-it)\frac{\lambda}{2}\hat{H}_0. \tag{80}$$

Second, we expand the squeeze operators in Taylor series and remain to first order in λ

$$\hat{S}^\dagger(\lambda) \approx 1 + \lambda\frac{((\hat{a}^\dagger)^2 - \hat{a}^2)}{8}, \tag{81}$$

and

$$\hat{S}_{\tilde{\omega}}(\lambda,t) \approx 1 + \lambda\frac{1}{8}\left[\hat{a}^2e^{-2it\omega} - (\hat{a}^\dagger)^2e^{2it\omega}\right], \tag{82}$$

to arrive to the expression

$$|\psi(t)\rangle \approx e^{-it\hat{H}_0}\left(1 + \frac{\lambda}{8}\left((\hat{a}^\dagger)^2(1-e^{2i\omega t}) + \hat{a}^2(e^{-2i\omega t}-1)\right) - \lambda\frac{it\omega}{2}\left(\hat{n}+\frac{1}{2}\right)\right)|\psi(0)\rangle, \tag{83}$$

which is the one obtained from the method introduced here.

5 The Dyson series in the matrix method

It is well known that in terms of the Dyson series [13–15], the wavefunctions of the perturbed problem are written as

$$|\psi(t)\rangle = e^{-i\hat{H}_0t}\hat{T}\left\{\exp\left[-i\lambda\int_0^t dt_1\hat{V}(t_1)\right]\right\}|\psi(0)\rangle, \tag{84}$$

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

$$\hat{T}[\hat{A}(t_1)\hat{B}(t_2)] = \begin{cases}\hat{B}(t_2)\hat{A}(t_1) \text{ if } t_2 > t_1,\\ \hat{A}(t_1)\hat{B}(t_2) \text{ if } t_1 > t_2.\end{cases} \tag{85}$$

On the other hand, from equation (55) we can write

$$|\psi(t)\rangle = \left(e^{-i\hat{H}_0t} + \sum_{n=1}^{\infty}\lambda^n\left(e^{-iMt}\right)_{(1,n+1)}\right)|\psi(0)\rangle; \tag{86}$$

so comparing equation (84) with equation (86), we derive the formula

$$\hat{T}\left\{\exp\left[-i\lambda\int_0^t dt_1\hat{V}(t_1)\right]\right\} = e^{i\hat{H}_0t}\sum_{n=0}^{\infty}\lambda^n\left(e^{-iMt}\right)_{(1,n+1)} \tag{87}$$

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

6 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 (57) 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 (34) and (53). 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 general expressions.

We would like to stress that this method allows easy application to any initial condition because it is based on an approximation to the evolution operator.

We have obtained the corrections to first order of the quadratic potential as perturbation to the harmonic oscillator. Finally, we have given an alternative expression for the Dyson series in a matrix form.

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