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Hamiltonian matrix representation of harmonic oscillator system with Linear-Cubic-Quartic (LCQ) perturbation

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Abstract. In this paper, we analyze the matrix representation of the energy operator (Hamiltonian) of the harmonic oscillator system when this system is perturbed by an LCQ perturbation. The LCQ perturbation is simultaneously acted on this system, so the total Hamiltonian is a summation of the pure oscillator harmonic operator term (in the annihilation and creation operator statement) and the three perturbation terms. In this work, we use three different small parameters for each term of the perturbation for keeping the generality. We use the simple algebraic method by using the Dirac notation and the well-known base vector of harmonic oscillator to analyze this problem. Next, we present every term of this operator in matrix representation and then adding them for finding matrix representation for the total Hamiltonian.

1. Introduction

The Harmonic Oscillator is a familiar topic in physics, be it classical physics, modern physics, or advanced physics. In fact, this topic is one of the most favorite topics to study so that it can be found in almost all fields of physics [1–8]. This means that this system plays a very important role in explaining various physical phenomena. This system has also been studied in mathematics both in a differentialintegral [9,10]; algebraic [11-13], and topological [5,14,15]. The rigorous study of physics and mathematics for more than one hundred years has confirmed it as one of the most important topics in the history of physics. However, on the other hand, the fact that this topic is still being studied means that there is still a lot to explore from this system.

As previously explained, the study of harmonic oscillators exists in various domains of physics, and quantum mechanics is no exception. The study of this topic is found in many parts, both pure harmonic oscillators and with the addition of perturbation terms, and various other forms of study. Like other subjects in physics, especially in advanced quantum mechanics, the harmonic oscillator studied, in general, is no longer in the study of pure harmonic oscillators, but has undergone modification ([15– 19]). Of course, these modifications are based on each of the physical phenomena studied. One of the modifications in the harmonic oscillator is when there is a spatial perturbation term, either linear, quadratic, cubic, or higher-order perturbation; even the combination of these perturbations in certain quantum systems.

One of the most widely used mathematical approaches to harmonic oscillators today is the algebraic approach, such as in the use of Dirac notation and matrix mechanics. The matrix representation of this type of quantum system becomes very interesting because the 'incarnate' formulation of the differentialintegral form as well as certain special functions such as the spherical harmonic function (which contains

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the Association's Legendre function) or the Laguerre function, can be represented in certain abstract notations by analysis simpler math.

In this paper, we perform an algebraic analysis of a harmonic oscillator with simultaneous perturbation of the linear, quadratic, and cubic terms. Our analysis is focused on finding a matrix representation form for the Hamiltonian operator of this system. To produce a more generalized representation of the matrix, we used three different small parameters for the three perturbation terms. Meanwhile, the base vector we use is the same as the base vector on standard harmonic oscillators. In closing this section, a little outline of this paper is as follows, first is an introduction, the second is about harmonic oscillators, and the third is about the representation of the Harmonic Oscillator Hamiltonian matrix with LCQ perturbation.

2. Harmonic Oscillator

As previously described, the harmonic oscillator plays a very important role in various fields of physics. For a harmonic oscillator quantum system, the Hamiltonian of the system can be written as [11,12]

$$\hat{H} = \frac{\hat{p}^2}{2m} + \frac{1}{2}m\omega^2 \hat{x}^2 \tag{1}$$

where \hat{x} is the position operator; $\hat{p} \equiv -i\hbar \left(\frac{d}{dx}\right)$, is the momentum operator; *m* is the mass of the particles, and is ω the classical angular oscillator frequency. Analysis of this system can be done analytically or algebraically, but in this paper, it will only be described algebraically using the Dirac operator method. Therefore, suppose equation (1) is written

$$\widehat{H} = \widehat{A}^2 + \widehat{B}^2 \tag{2}$$

where $\hat{A}^2 = \frac{1}{2}m\omega^2 \hat{x}^2$; dan $\hat{B}^2 = \frac{\hat{p}^2}{2m}$. Because \hat{A} and \hat{B} do not commute, equation (2) can be written $\hat{H} = (\hat{A} + i\hat{B})(\hat{A} - i\hat{B}) - i[\hat{B}, \hat{A}].$ (3)

where $[\hat{B}, \hat{A}] = -\frac{i\hbar\omega}{2}$. Then, equation (3) becomes

$$\widehat{H} = \left(\omega \sqrt{\frac{m}{2}}\,\widehat{x} + i\frac{\widehat{p}}{\sqrt{2m}}\right) \left(\omega \sqrt{\frac{m}{2}}\,\widehat{x} - i\frac{\widehat{p}}{\sqrt{2m}}\right) - \frac{\hbar\omega}{2}.\tag{4}$$

By performing several algebraic steps, it is obtained

$$\widehat{H} = \hbar\omega \left(\left(\sqrt{\frac{m\omega}{2\hbar}} \, \hat{x} + i \frac{\hat{p}}{\sqrt{2m\hbar\omega}} \right) \left(\sqrt{\frac{m\omega}{2\hbar}} \, \hat{x} - i \frac{\hat{p}}{\sqrt{2m\hbar\omega}} \right) - \frac{1}{2} \right). \tag{5}$$

Or, equation (5) can also be written as

$$\widehat{H} = \hbar \omega \left(\widehat{a} \widehat{a}^{\dagger} - \frac{1}{2} \right). \tag{6}$$

where \hat{a} and \hat{a}^{\dagger} are annihilation and creation operator, respectively, by definition

$$\hat{a} \equiv \sqrt{\frac{m\omega}{2\hbar}} \,\hat{x} + i \frac{\hat{p}}{\sqrt{2m\hbar\omega}} \quad ; \quad \hat{a}^{\dagger} \equiv \sqrt{\frac{m\omega}{2\hbar}} \,\hat{x} - i \frac{\hat{p}}{\sqrt{2m\hbar\omega}}. \tag{7}$$

Because $[\hat{a}, \hat{a}^{\dagger}] = 1$, equation (6) can also be written

$$\hat{H} = \hbar\omega \left(\hat{a}^{\dagger} \hat{a} + \frac{1}{2} \right). \tag{8}$$

Furthermore, if a harmonic oscillator state is defined as $\phi_n \equiv |n\rangle$,

(9) where this state satisfies the orthogonality characteristic $\langle n'|n\rangle = \delta_{n'n}$; where $\delta_{n'n}$ is the Kronecker delta function. Because [11]

$$\hat{a}|n\rangle = \sqrt{n}|n\rangle \,\,\mathrm{dan} \,\,\hat{a}^{\dagger}|n\rangle = \sqrt{n+1}|n\rangle,$$
(10)

then

$$\hat{a}^{\dagger}\hat{a}|n\rangle = n|n\rangle. \tag{11}$$

Based on equation (11), we define a new operator, namely the number operator $\hat{N} \equiv \hat{a}^{\dagger} \hat{a}$, so that equation (8) becomes

$$\widehat{H} = \hbar\omega \left(\widehat{N} + \frac{1}{2}\right). \tag{12}$$

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If operator \hat{H} is worked on state $|n\rangle$ then $\hat{H}|n\rangle = E_n|n\rangle$, where $E_n = \hbar\omega\left(n + \frac{1}{2}\right)$, where n = 0, 1, 2, ...We can apply the creation operator to state $|0\rangle$ consecutively to get the state to a particular $|n\rangle$, namely

$$|n\rangle = \left(\frac{\left(\hat{a}^{\dagger}\right)^{n}}{\sqrt{n!}}\right)|0\rangle. \tag{13}$$

From equation (10) and using the orthonormality conditions for $\{|n\}$, the elements of the matrix representation for the operators \hat{a} and \hat{a}^{\dagger} are

 $\langle n'|\hat{a}|n\rangle = \sqrt{n}\delta_{n',n-1}$; $\langle n'|\hat{a}^{\dagger}|n\rangle = \sqrt{n+1}\delta_{n',n+1}$. (14) Based on equation (7), it is obtained

$$\hat{x} = \sqrt{\frac{\hbar}{2m\omega}} (\hat{a} + \hat{a}^{\dagger}); \quad \hat{p} = -i \sqrt{\frac{m\hbar\omega}{2}} (\hat{a} - \hat{a}^{\dagger}).$$
(15)

Therefore, the elements of the matrix representation for \hat{x} and \hat{p} are

$$\langle n'|\hat{x}|n\rangle = \sqrt{\frac{\hbar}{2m\omega}} \left(\sqrt{n}\delta_{n',n-1} + \sqrt{n+1}\delta_{n',n+1}\right) , \qquad (16)$$

$$\langle n'|\hat{p}|n\rangle = -i \sqrt{\frac{m\hbar\omega}{2}} \left(\sqrt{n}\delta_{n',n-1} - \sqrt{n+1}\delta_{n',n+1}\right) \,. \tag{17}$$

3. Matrix Representation

This system is a harmonic oscillator system with LCQ perturbation. The Hamiltonian form of this system is

$$\hat{H} = \frac{\hat{p}^2}{2m} + \frac{1}{2}m\omega^2\hat{x}^2 + \alpha\hat{x} + \beta\hat{x}^3 + \gamma\hat{x}^4$$
(18)

where α , β , and γ have different units, and each of these constants has a definition

$$\alpha = \lambda_1 \omega \sqrt{2m\omega\hbar}; \ \beta = \lambda_2 \left(\frac{2m\omega^{\frac{5}{3}}}{\hbar^{\frac{1}{3}}}\right)^{3/2}; \ \gamma = \lambda_3 \frac{4m^2 \omega^3}{\hbar}, \tag{19}$$

where λ_1, λ_2 , and λ_3 are small parameters. Especially for the first term and the second term on the right side of equation (18), we can express it in the form of ladder operators \hat{a} and \hat{a}^{\dagger} , where there is a relationship

$$\hat{x} = \sqrt{\frac{\hbar}{2m\omega}} (\hat{a} + \hat{a}^{\dagger}).$$
⁽²⁰⁾

So that equation (18) can also be expressed in terms of

$$\widehat{H} = \hbar\omega \left(\widehat{a}^{\dagger} \widehat{a} + \frac{1}{2} \right) + \alpha \widehat{x} + \beta \widehat{x}^3 + \gamma \widehat{x}^4$$
(21)

It should be noted that the term $\hbar\omega(\hat{a}^{\dagger}\hat{a} + \frac{1}{2})$ is a pure harmonic oscillator operator, while the three extra terms to the right are the perturbation terms.

Now we start creating a matrix representation of each operator. The basis used in this analysis is the base of the harmonic oscillator, namely [20]

$$|0\rangle \doteq \begin{pmatrix} 1\\0\\0\\0\\\vdots \end{pmatrix}; |1\rangle \doteq \begin{pmatrix} 0\\1\\0\\0\\\vdots \end{pmatrix}; |2\rangle \doteq \begin{pmatrix} 0\\0\\1\\0\\\vdots \end{pmatrix}; \dots$$
(22)

First, we compute the matrix representation of the operator \hat{a} , with the matrix elements a_{mn} , namely $a_{mn} = \langle m | \hat{a} | n \rangle = \sqrt{n} \delta_{m,n-1}$ (23)

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where $\hat{a}|n\rangle = \sqrt{n}|n-1\rangle$. Using the basis of equation (22), it is obtained

$$\hat{a} \doteq \begin{pmatrix} 0 & 1 & 0 & 0 & 0 & \dots \\ 0 & 0 & \sqrt{2} & 0 & 0 & \dots \\ 0 & 0 & 0 & \sqrt{3} & 0 & \dots \\ 0 & 0 & 0 & 0 & 2 & \dots \\ 0 & 0 & 0 & 0 & 0 & \dots \\ \vdots & \vdots & \vdots & \vdots & \vdots & \ddots \end{pmatrix}.$$
(24)

Next, we compute the matrix representation for the operator \hat{a}^{\dagger} , with the matrix elements a_{mn}^{\dagger} , i.e. $a_{mn}^{\dagger} = \langle m | \hat{a}^{\dagger} | n \rangle = \sqrt{n+1} \delta_{m,n+1}$ where $\hat{a}^{\dagger} | n \rangle = \sqrt{n+1} | n+1 \rangle$. Hence, the matrix representation of the operator \hat{a}^{\dagger} is obtained (25)

$$\hat{a}^{\dagger} \doteq \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & \dots \\ 1 & 0 & 0 & 0 & 0 & \dots \\ 0 & \sqrt{2} & 0 & 0 & 0 & \dots \\ 0 & 0 & \sqrt{3} & 0 & 0 & \dots \\ 0 & 0 & 0 & 2 & 0 & \dots \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \ddots \end{pmatrix}.$$
(26)

By obtaining the matrix representation \hat{a} and \hat{a}^{\dagger} , it can be easily calculated the representation of a pure harmonic oscillator matrix which has the matrix equation $\hat{H}_0 = \hbar \omega (\hat{a}^{\dagger} \hat{a} + \frac{1}{2} \hat{l})$, where \hat{l} is an identity matrix that corresponds to the matrix order \hat{a} and \hat{a}^{\dagger} . Before proceeding to the part of the perturbation terms, it is good to present a representation of the Hamiltonian matrix of a pure harmonic oscillator, namely 4 10 ^

$$\widehat{H}_{0} \doteq \hbar \omega \begin{pmatrix} 1/2 & 0 & 0 & 0 & 0 & \dots \\ 0 & 3/2 & 0 & 0 & 0 & \dots \\ 0 & 0 & 5/2 & 0 & 0 & \dots \\ 0 & 0 & 0 & 7/2 & 0 & \dots \\ 0 & 0 & 0 & 0 & 9/2 & \dots \\ \vdots & \vdots & \vdots & \vdots & \vdots & \ddots \end{pmatrix}.$$

$$(27)$$

Now, we come to the perturbation terms. First, we calculate the linear term, which is the matrix representation for \hat{x} . Based on equation (20), the element of the operator matrix \hat{x} is

$$x_{mn} = \langle m | \hat{x} | n \rangle = \sqrt{\frac{\hbar}{2m\omega}} \left(\sqrt{n} \delta_{m,n-1} + \sqrt{n+1} \delta_{m,n+1} \right)$$
(28)

So that the matrix representation is obtained, namely

$$\hat{x} \doteq \sqrt{\frac{\hbar}{2m\omega}} \hat{A}_1 \tag{29}$$

where

$$\hat{A}_{1} \doteq \begin{pmatrix} 0 & 1 & 0 & 0 & 0 & 0 & \dots \\ 1 & 0 & \sqrt{2} & 0 & 0 & 0 & \dots \\ 0 & \sqrt{2} & 0 & \sqrt{3} & 0 & 0 & \dots \\ 0 & 0 & \sqrt{3} & 0 & 2 & 0 & \dots \\ 0 & 0 & 0 & 2 & 0 & \sqrt{5} & \dots \\ 0 & 0 & 0 & \sqrt{5} & 0 & \dots \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \ddots \end{pmatrix}.$$
(30)

Next, we compute the matrix representation for the cubic perturbation term. Based on the form of the operator in equation (20), the matrix representation form of the \hat{x}^3 operator can be calculated by first calculating the x_{mn}^3 matrix elements,

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$$\begin{aligned} x_{mn}^{3} &= \langle m | \hat{x}^{3} | n \rangle \\ &= \left(\frac{\hbar}{2m\omega} \right)^{\frac{3}{2}} \left(\sqrt{n(n-1)(n-2)} \delta_{m,n-3} + 3n\sqrt{n} \delta_{m,n-1} \right. \\ &+ 3(n+1)\sqrt{n+1} \delta_{m,n+1} + \sqrt{(n+1)(n+2)(n+3)} \delta_{m,n+3} \right). \end{aligned}$$
(31)

Equation (31) can easily be obtained by working on the operator in equation (20) three times in a row against base $|n\rangle$, followed by working on $\langle m|$ from the left side against the results of the previous operation. Briefly, it can be shown as follows

$$\hat{x}^{3}|n\rangle = \hat{x}^{2}(\hat{x}|n\rangle) = \hat{x}^{2} \left(\frac{\hbar}{2m\omega} \left(\sqrt{n}|n-1\rangle + \sqrt{n+1}|n+1\rangle\right)\right),\tag{32}$$

then,

$$\hat{x}^{3}|n\rangle = \hat{x}\left(\sqrt{\frac{\hbar}{2m\omega}}\left(\sqrt{n}|n-1\rangle + \sqrt{n+1}|n+1\rangle\right)\right).$$
(33)

Finally, it is obtained

$$\hat{x}^{3}|n\rangle = \left(\frac{\hbar}{2m\omega}\right)^{\frac{3}{2}} \left(\sqrt{n(n-1)(n-2)}|n-3\rangle + 3n\sqrt{n}|n-1\rangle + 3(n+1)\sqrt{n+1}|n+1\rangle + \sqrt{(n+1)(n+2)(n+3)}|n+3\rangle\right).$$
(34)

By multiplying $\langle m |$ from the left side of equation (34), we get equation (31). Referring to equation (31), the matrix representation of the operator \hat{x}^3 is

$$\hat{x}^3 \doteq \left(\frac{\hbar}{2m\omega}\right)^{\frac{3}{2}} \hat{A}_2,\tag{35}$$

where

$$\hat{A}_{2} \doteq \begin{pmatrix} 0 & 3 & 0 & \sqrt{6} & 0 & 0 & \dots \\ 3 & 0 & 6\sqrt{2} & 0 & 2\sqrt{6} & 0 & \dots \\ 0 & 6\sqrt{2} & 0 & 9\sqrt{3} & 0 & 2\sqrt{15} & \dots \\ \sqrt{6} & 0 & 9\sqrt{3} & 0 & 24 & 0 & \dots \\ 0 & 2\sqrt{6} & 0 & 24 & 0 & 15\sqrt{5} & \dots \\ 0 & 0 & 2\sqrt{15} & 0 & 15\sqrt{5} & 0 & \dots \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \ddots \end{pmatrix}.$$
(36)

Next, we compute the matrix representation for the quartic perturbation term. To obtain a matrix representation of the \hat{x}^4 operator, it is done in the following way

$$\hat{x}^4 |n\rangle = \hat{x}(\hat{x}^3 |n\rangle)$$

$$= \hat{x} \left(\left(\frac{\hbar}{2m\omega} \right)^{\frac{3}{2}} \left(\sqrt{n(n-1)(n-2)} |n-3\rangle + 3n\sqrt{n} |n-1\rangle + 3(n+1)\sqrt{n+1} |n+1\rangle + \sqrt{(n+1)(n+2)(n+3)} |n+3\rangle \right) \right)$$
(37)

It can be seen that the form $\hat{x}^3 | n \rangle$ in equation (37) is taken from equation (34). Then, equation (37) becomes

$$\hat{x}^{4}|n\rangle = \left(\frac{\hbar}{2m\omega}\right)^{2} \left(\sqrt{n(n-1)(n-2)(n-3)}|n-4\rangle + 2(2n-1)\sqrt{n(n-1)}|n-2\rangle + 3(2n^{2}+2n+1)|n\rangle + 2(2n+3)\sqrt{(n+1)(n+2)}|n+2\rangle + \sqrt{(n+1)(n+2)(n+3)(n+4)}|n+4\rangle\right).$$
(38)

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By multiplying $\langle m |$ from the left side with respect to equation (38), it is obtained $x_{mn}^4 = \langle m | \hat{x}^4 | n \rangle$

$$= \left(\frac{\hbar}{2m\omega}\right)^{2} \left(\sqrt{n(n-1)(n-2)(n-3)}\delta_{m,n-4} + 2(2n-1)\sqrt{n(n-1)}\delta_{m,n-2} + 3(2n^{2}+2n+1)\delta_{m,n} + 2(2n+3)\sqrt{(n+1)(n+2)}\delta_{m,n+2} + \sqrt{(n+1)(n+2)(n+3)(n+4)}\delta_{m,n+4}\right).$$
(39)

Based on equation (39), the \hat{x}^4 operator matrix representation is obtained as follows

$$\hat{x}^4 \doteq \left(\frac{\hbar}{2m\omega}\right)^2 \hat{A}_3,\tag{40}$$

where

$$\hat{A}_{3} \doteq \begin{pmatrix} 3 & 0 & 6\sqrt{2} & 0 & 2\sqrt{6} & 0 & \dots \\ 0 & 15 & 0 & 10\sqrt{6} & 0 & 2\sqrt{30} & \dots \\ 6\sqrt{2} & 0 & 39 & 0 & 28\sqrt{3} & 0 & \dots \\ 0 & 10\sqrt{6} & 0 & 75 & 0 & 36\sqrt{5} & \dots \\ 2\sqrt{6} & 0 & 28\sqrt{3} & 0 & 123 & 0 & \dots \\ 0 & 2\sqrt{30} & 0 & 36\sqrt{5} & 0 & 183 & \dots \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \ddots \end{pmatrix}.$$

$$(41)$$

Now we compute the matrix representation of the total Hamiltonian of the system. By using the forms in equation (19), equation (21) in the form of a matrix equation can be written

$$\widehat{H} \doteq \hbar \omega \widehat{\eta} \tag{42}$$

where

$$\hat{\eta} \doteq \hat{a}^{\dagger} \hat{a} + \frac{1}{2} \hat{l} + \lambda_1 \hat{A}_1 + \lambda_2 \hat{A}_2 + \lambda_3 \hat{A}_3.$$
(43)

By using equations (24), (26), (30), (36), (41), and of course the corresponding identity matrices, equation (43) in the matrix representation can be written explicitly

$$\hat{\eta} \doteq \begin{pmatrix} \frac{1}{2} + 3\lambda_3 & \lambda_1 + 3\lambda_2 & 6\sqrt{2}\lambda_3 & \sqrt{6}\lambda_2 & 2\sqrt{6}\lambda_3 & 0 & \dots \\ \lambda_1 + 3\lambda_2 & \frac{3}{2} + 15\lambda_3 & \sqrt{2}\lambda_1 + 6\sqrt{2}\lambda_2 & 10\sqrt{6}\lambda_3 & 2\sqrt{6}\lambda_2 & 2\sqrt{30}\lambda_3 & \dots \\ 6\sqrt{2}\lambda_3 & \sqrt{2}\lambda_1 + 6\sqrt{2}\lambda_2 & \frac{5}{2} + 39\lambda_3 & \sqrt{3}\lambda_1 + 9\sqrt{3}\lambda_2 & 28\sqrt{3}\lambda_3 & 2\sqrt{15}\lambda_2 & \dots \\ \sqrt{6}\lambda_2 & 10\sqrt{6}\lambda_3 & \sqrt{3}\lambda_1 + 9\sqrt{3}\lambda_2 & \frac{7}{2} + 75\lambda_3 & 2\lambda_1 + 24\lambda_2 & 36\sqrt{5}\lambda_3 & \dots \\ 2\sqrt{6}\lambda_3 & 2\sqrt{6}\lambda_2 & 28\sqrt{3}\lambda_3 & 2\lambda_1 + 24\lambda_2 & \frac{9}{2} + 123\lambda_3 & \sqrt{5}\lambda_1 + 15\sqrt{5}\lambda_2 & \dots \\ 0 & 2\sqrt{30}\lambda_3 & 2\sqrt{15}\lambda_2 & 36\sqrt{5}\lambda_3 & \sqrt{5}\lambda_1 + 15\sqrt{5}\lambda_2 & \dots \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \ddots \end{pmatrix}$$

$$(44)$$

Based on equations (42) and (44), if we choose all perturbation parameters $\lambda_1 = \lambda_2 = \lambda_3 = 0$, then the Hamiltonian of the system will return to the form of Hamiltonian of a pure harmonic oscillator, as shown in equation (27).

4. Conclusion

We have performed calculations to obtain a representation of the Hamiltonian matrix for a harmonic oscillator quantum system with linear-cubic-quartic perturbation. This matrix representation contains three different parameters for each perturbation term. By selecting a state when all these parameters are zero (without perturbation), the matrix representation will be reduced to the Hamiltonian for a pure harmonic oscillator. One thing to note is that this matrix has an infinite order because, for the case of the harmonic oscillator, we use the basis as shown in equation (22), which those allow us to display more matrix elements than is shown in equation (44). However, the matrix elements shown in equation

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(44) are very representative to see the effect of the simultaneous presence of the first, third, and fourthorder perturbations on this quantum system. Of course, we will have different forms of elements if the perturbation applied to the system has a different combination, for example, if the perturbation is of the order of one, two, and three simultaneously; three, four, and five; or any other possible combinations.

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