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# Generalized quantum anharmonic oscillator using an operator ordering approach

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**Abstract.** We construct a generalized expression for the normal ordering of $(a+a^\dagger)^m$ for integral values of $m$ and use the result to study the quantum anharmonic oscillator problem in the Heisenberg approach. In particular, we derive generalized expressions for energy eigenvalues and frequency shifts for the Hamiltonian $H = \frac{x^2}{2} + \frac{\dot{x}^2}{2} + \frac{\lambda}{m}x^m$. We also derive a closed-form first-order multiscale perturbation theoretic operator solution of this Hamiltonian with a view to generalize some recent results of Bender and Bettencourt (1996 *Phys. Rev. Lett.* **77** 4114, 1996 *Phys. Rev.* D **54** 1710).

## 1. Introduction

The simple harmonic oscillator (SHO) model can be used to understand a wide variety of physical phenomena ranging from problems in Newtonian mechanics to those in quantum field theory. This solvable model describes a small oscillation of a system about the mean position of equilibrium under the action of a linear restoring force. However, for a real physical problem one has to incorporate the anharmonicity in the model Hamiltonian. In this case the equation of motion is not exactly solvable and, in fact, the anharmonic oscillators (AHOs) provide one of the simplest examples of quantum mechanical systems which cannot be solved without making use of approximation techniques. This was why the AHO problem received considerable attention from physicists and mathematicians from the very beginning of the subject. It is an outstanding curiosity to note that studies in the AHO problems have enriched the subject of large-order perturbation theory [1–5], divergent expansion of quantum mechanics [6, 7], Laplace transformation representation of energy eigenvalues [8–12], computational physics and Pade and Borel summation of perturbation series [13].

In this paper we shall study the generalized quantum AHO problem in the Heisenberg representation by making use of two simple normal ordering theorems we have derived for the expansion of $(a+a^\dagger)^m$. We shall see that the merit of this paper is its simplicity. For example, the present method provides, on the one hand, a straightforward mathematical framework to construct expressions for the energy eigenvalues as well as frequency shifts and, on the other hand, generalizes some of the recent results on the topic by Bender and Bettencourt [14, 15].

The Hamiltonian of a generalized AHO having unit mass and unit frequency is written as

$$H = H_0 + \frac{\lambda}{m}x^m = \frac{x^2}{2} + \frac{\dot{x}^2}{2} + \frac{\lambda}{m}x^m \tag{1}$$

with

$$x = \frac{1}{\sqrt{2}}(a^\dagger + a). \tag{2}$$

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Here we have chosen to work in units in which $\hbar = 1$. The equation of motion corresponding to (1) is

$$\ddot{x} + x + \lambda x^{m-1} = 0. \tag{3}$$

Equation (3) cannot be solved exactly for $m > 2$. However, a large number of approximation methods are available for solving (3) for particular values of $m$. These include the perturbation technique [16], variation of parameters and the Taylor series approach [17]. Ordinary perturbation technique leads to the unwanted secular terms that grow rapidly with time. Secular terms are unwanted because they are in conflict with the physical requirement that the solution be finite. There are some methods which are successfully used to sum up the secular terms for all orders. Multiscale perturbation theory (MSPT) is one of those methods [14–16].

The AHO problem can be approached in two different ways in quantum mechanics. One way is the c-number approach or the Schrödinger approach and the other way is the operator approach or the Heisenberg approach. In the Schrödinger approach the wave functions and/or the state vectors are time dependent while the operators characterizing the quantum system are time independent. This approach is used to solve the quantum AHO problem as eigenvalue problem. In these problems, energy eigenvalues are expressed as the sum of different orders of the anharmonic constant. As opposed to this, the operators carry the time dependence in the Heisenberg approach and the state vectors are time-independent. In this approach, we solve the Heisenberg equation of motion to obtain the time development of the position operator.

There is an extensive amount of literature on the c-number approach [1–13, 18] but the situation is different for the Heisenberg approach because the complicated operator algebra tends to pose serious mathematical problems. Our main objective in this work is to provide a theoretical framework which is free from calculational difficulties. The first operator solution of a quantum oscillator was given by Bender and Bettencourt [14, 15] using MSPT. They generalized the existing theory of MSPT into an operator approach to obtain the zeroth-order solution involving a quantum operator analogue of the classical first-order frequency shift and interpreted it as an operator mass renormalization that expresses the first-order shift of all energy levels. Somewhat later Mandal [19] approached the problem (up to first order) using the Taylor series method. All these solutions were found for the quartic oscillator only. Application of the Taylor series method to sextic and octic oscillator problems are now in order [20].

The Schroedinger approach to the AHO problem in quantum mechanics has made a significant contribution to the development of the perturbative techniques we use today but the suitability of the other approach (the Heisenberg approach) has not yet been studied in detail. To date we have no operator solutions of higher AHOs although these might be relevant to various physical problems. Keeping these in mind, we will suggest a novel method in which MSPT results for AHOs in general can be found. To that end we prove in section 2 two theorems to construct a normal ordered expansion of $(a + a^\dagger)^m$. We obtain a generalized expression for the energy eigenvalues in section 3. We devote section 4 to constructing a generalized solution for the equation of motion (3) and specialize our result to reproduce some of the existing results as useful checks on the generalized solution we have obtained.

## 2. Operator ordering theorems

On very general grounds one knows that in quantum mechanics and quantum field theory proper ordering of the operators plays a crucial role. Let $f(a, a^\dagger)$ be an arbitrary operator function of the usual bosonic annihilation and creation operators $a$ and $a^\dagger$, which satisfy the

commutation relation

$$[a, a^\dagger] = 1. \tag{4}$$

One can write $f(a, a^\dagger)$ in such a way that all powers of $a^\dagger$ always appear to the left of all powers of $a$. Then $f(a, a^\dagger)$ is said to be normal ordered. In this paper we want to write $(a + a^\dagger)^m$ in the normal ordered form for integral values of $m$. Traditionally for a given value of $m$ this is achieved by using a very lengthy procedure which involves repeated application of (4). One of our objectives in this work is to construct a normal ordered expansion of $(a + a^\dagger)^m$ without taking recourse to such repeated applications.

We shall denote the normal ordered form of $f$ by $f_{\mathrm{N}}$. On the other hand $: f :$ will denote an operator obtained from $f$ by arranging all powers of $a^\dagger$ to the left of all powers of $a$ without making use of the commutation relation in (4). Now if $f = aa^\dagger$ then $f_{\mathrm{N}} = a^\dagger a + 1$ and $: f := a^\dagger a$. Therefore, we can write

$$: (a + a^\dagger)^m :=: (a^\dagger + a)^m := a^m +^m C_1 a^\dagger a^{m-1} + \cdots +^m C_r a^{\dagger r} a^{m-r} + \cdots + a^{\dagger m}. \tag{5}$$

Thus in this notation $: (a + a^\dagger)^m :$ is simply a binomial expansion in which powers of the $a^\dagger$ are always kept to the left of the powers of the $a$. To write $(a^\dagger + a)^m_{\mathrm{N}}$ we shall proceed by using the following theorems.

**Theorem 1.**

$$: (a^\dagger + a)^m : (a^\dagger + a) =: (a^\dagger + a)^{m+1} : + m : (a^\dagger + a)^{m-1} : . \tag{6}$$

**Proof.** From (5) $: (a^\dagger + a)^m : (a^\dagger + a)$ can be written in the form

$$\begin{aligned} &: (a^\dagger + a)^m : (a^\dagger + a) \\ &\quad = [a^{\dagger m+1} + (^m C_1 +^m C_0) a^{\dagger m} a + (^m C_2 +^m C_1) a^{\dagger m-1} a^2 \\ &\qquad + \cdots + (^m C_r +^m C_{r-1}) a^{\dagger m-r+1} a^r + \cdots] \\ &\qquad + (^m C_1 a^{\dagger m-1} + 2\,^m C_2 a^{\dagger m-2} a + \cdots + r\,^m C_r a^{\dagger m-r} a^{r-1} + \cdots). \end{aligned} \tag{7}$$

□

The theorem in (6) can be obtained by simply using the following identities in the above:

$$\begin{aligned} &(a^r a^\dagger)_{\mathrm{N}} = a^\dagger a^r + r a^{r-1} \\ &r\,^n C_r = n\,^{n-1} C_{r-1} \\ &^{m+1} C_{r+1} = (^m C_r +^m C_{r+1}). \end{aligned} \tag{8}$$

Note that the first identity in (8) can be proved with the help of the general operator ordering theorems [21] while the other two are trivial.

**Theorem 2.** *For any integral values of m*

$$(a^\dagger + a)^m_{\mathrm{N}} = \sum_{r=0,2,4,\ldots}^{m} t_r\,^m C_r : (a^\dagger + a)^{m-r} : \tag{9}$$

*with*

$$t_r = \frac{(r-1)!}{2^{(\frac{r}{2}-1)}(\frac{r}{2}-1)!} \qquad \textit{for} \qquad r \geqslant 4 \tag{10}$$

*and*

$$t_0 = t_2 = 1. \tag{11}$$

**Proof.** Using theorem 1, we can write

$$\begin{aligned}
&(a^\dagger + a)_{\rm N} =: (a^\dagger + a) : \\
&(a^\dagger + a)^2_{\rm N} =: (a^\dagger + a)^2 : +1 \\
&(a^\dagger + a)^3_{\rm N} =: (a^\dagger + a)^3 : +3 : (a^\dagger + a) : \\
&(a^\dagger + a)^4_{\rm N} =: (a^\dagger + a)^4 : +6 : (a^\dagger + a)^2 : +3 \\
&(a^\dagger + a)^5_{\rm N} =: (a^\dagger + a)^5 : +10 : (a^\dagger + a)^3 : +15 : (a^\dagger + a) : \\
&\cdots \qquad \cdots \qquad \cdots \\
&\cdots \qquad \cdots \qquad \cdots \\
&\cdots \qquad \cdots \qquad \cdots \\
&(a^\dagger + a)^9_{\rm N} =: (a^\dagger + a)^9 : +36 : (a^\dagger + a)^7 : +378 : (a^\dagger + a)^5 : \\
&\qquad\qquad +1260 : (a^\dagger + a)^3 : +945 : (a^\dagger + a) : .
\end{aligned} \tag{12}$$

From (12) we venture to identify the general form of the above expansion for a given value of $m$ as

$$(a^\dagger + a)^m_{\rm N} = \sum_{r=0,2,4,\ldots}^{m} t_r{}^m C_r : (a^\dagger + a)^{m-r} : . \tag{13}$$

It is easy to check that (13) gives all the expansions of (12) such that (13) is true for $m = 1, 2, \ldots, 9$. The general validity of (13) can be ensured by using the method of induction. This establishes that (13) gives the normal ordered expansion of $(a^\dagger + a)^m$ for any arbitrary integer $m$. We shall now use this normal ordered expansion to study the anharmonic oscillator problem. □

## 3. Energy eigenvalues

The first-order energy eigenvalue $E_1$ is $\langle n|H|n\rangle$, where $|n\rangle$ is the number state. In the literature there are two lengthy procedures [22] to obtain $E_1$. The first one is the usual normal ordering method. This method involves iterative use of (4) and the number of iterations increases very quickly as $m$ increases. For a given value of $m$ we need $[2^m - (m + 1)]$ iterations. This shows that for large $m$ the construction of the expansion $(a^\dagger + a)^m_{\rm N}$ becomes formidable. In the second procedure one proceeds by making repeated applications of the $x$ operator to the number state. This procedure is as lengthy as the normal ordering method. In the following we implement theorem 2 to derive an uncomplicated method to construct an expansion for $E_1$ for the Hamiltonian (1).

Using the result in (9) we can write the expression for $E_1$ for any integer value of $m$ in the form

$$\begin{aligned}
E_1 &= \left(n + \frac{1}{2}\right) + \frac{\lambda}{2^{\frac{m}{2}} m} \langle n| \sum_{r=0,2,4,\ldots}^{m} t_r{}^m C_r : (a^\dagger + a)^{m-r} : |n\rangle \\
&= \left(n + \frac{1}{2}\right) + \frac{\lambda}{2^{\frac{m}{2}} m} \langle n| \sum_{r=0,2,4,\ldots}^{m} t_r{}^m C_r{}^{m-r} C_{\frac{m-r}{2}} a^{\dagger\,\frac{m-r}{2}} a^{\frac{m-r}{2}} |n\rangle \\
&= \left(n + \frac{1}{2}\right) + \frac{\lambda}{2^{\frac{m}{2}} m} \sum_{r=0,2,4,\ldots}^{m} t_r{}^m C_r{}^{m-r} C_{\frac{m-r}{2}}{}^n \, C_{\frac{m-r}{2}} \left(\frac{m-r}{2}\right)!.
\end{aligned} \tag{14}$$

The expression (14) involves summations which are easy to evaluate and thereby avoids the difficulties associated with earlier iterative procedures. Although somewhat forced, it may be tempting to compare the simplicity sought in our approach with the use of logarithms in a

numerical calculation or use of integral transforms in solving a partial differential equation. It is of interest to note that an expression similar to (14) can also be constructed for the first-order energy eigenvalue of a Hamiltonian in which the anharmonic term is a polynomial in $x$. This type of Hamiltonian is very frequently used in nonlinear optics.

## 4. MSPT solution of the generalized quantum AHO

We want to obtain the MSPT operator solution of equation (3) for arbitrary integral values of $m$. The essential idea behind our approach is that the quantum operator analogue of the classical first-order frequency shift is an operator function ($\Omega(H_0)$) of the unperturbed Hamiltonian $H_0$ and secondly a correct solution should reproduce the first-order energy spectrum. Now the general form of the zeroth-order solution of (3) is given by

$$x_0(t) = \frac{1}{G(n)}[x(0)\cos(t+\lambda\Omega(H_0)t) + \cos(t+\lambda\Omega(H_0)t)x(0) + \dot{x}(0)\sin(t+\lambda\Omega(H_0)t) + \sin(t+\lambda\Omega(H_0)t)\dot{x}(0)] \tag{15}$$

where $G(n)$ is a normalization factor. So our task is to find $\Omega(H_0)$ and $G(n)$ in general. From equation (14) we obtain the energy difference for two consecutive energy levels as

$$\begin{aligned}\omega_{n,n-1} &= (E_1)_{m,n} - (E_1)_{m,n-1} \\ &= 1 + \lambda\omega(m,n) \\ &= 1 + \frac{\lambda}{2^{\frac{m}{2}}m}\sum_{r=0,2,4,\ldots}^{(m-2)} t_r\, {}^{m}C_r\, {}^{m-r}C_{\frac{m-r}{2}}\, {}^{n-1}C_{\frac{m-r-2}{2}} \left(\frac{m-r}{2}\right)!. \end{aligned} \tag{16}$$

Since the correct quantum operator solution has to give the first-order energy spectrum, we should have

$$\langle n-1|x_0(t)|n\rangle = \langle n-1|x_0(0)|n\rangle\cos[t+\lambda\omega(m,n)t] + \langle n-1|p_0(0)|n\rangle\sin[t+\lambda\omega(m,n)t]. \tag{17}$$

Equations (15) and (17) impose restrictions on our unknown functions $\Omega(H_0)$ and $G(n)$. The condition imposed on $\Omega(H_0)$ is

$$\langle n|\Omega(H_0)|n\rangle + \langle n-1|\Omega(H_0)|n-1\rangle = 2\omega(m,n) \tag{18}$$

or

$$\Omega(n+\tfrac{1}{2}) + \Omega(n-\tfrac{1}{2}) = 2\omega(m,n). \tag{19}$$

For a particular $m$ the right-hand side is a known polynomial in $n$ and our job is simply to find $\Omega(n+\frac{1}{2})$. We obtain this as

$$\Omega\left(n+\frac{1}{2}\right) = 2\left[\sum_{k=0}^{n}(-1)^{n-k}\omega(m,k)\right] + (-1)^{n+\frac{m}{2}}\frac{t_m}{2^{\frac{m-2}{2}}m}. \tag{20}$$

Substituting the functional form of $\Omega(n+\frac{1}{2})$ or $\Omega(H_0)$ in (15) if we impose condition (17) we will obtain

$$G(n) = 2\cos\left[\frac{\lambda t}{2}\left(\Omega\left(n+\frac{1}{2}\right) - \Omega\left(n-\frac{1}{2}\right)\right)\right]. \tag{21}$$

The results in (20) and (21) when substituted in (15) solve the generalized quantum AHO problem.

*4.1. Specific results and their comparison with the existing spectra*

Although we have solved the quantum AHO in general, it is not possible to compare our solution directly with other existing results since the present study happens to be the first operator solution of the generalized AHO. There are methods to calculate the first-order classical frequency shift for particular $m$ in the appropriate classical limit ($x(0) = a, \dot{x}(0) = 0$). Here we calculate some specific results from our general expressions and compare them with the existing results.

For $m = 4$ we have

$$\Omega\left(n + \frac{1}{2}\right) = \frac{3n}{4} + \frac{3}{8} = \frac{3}{4}\left(n + \frac{1}{2}\right). \tag{22}$$

Therefore,

$$\Omega(H_0) = \tfrac{3}{4}H_0 \qquad \text{and} \qquad G(n) = 2\cos\left(\frac{3\lambda t}{8}\right). \tag{23}$$

In terms of (23) the total solution for the quantum quartic AHO is

$$\begin{aligned} x(t)|_{m=4} = {} & \frac{1}{2\cos(\frac{3\lambda t}{8})}\left[x(0)\cos\left[t + \frac{3\lambda t}{4}H_0\right] + \cos\left[t + \frac{3\lambda t}{4}H_0\right]x(0)\right. \\ & \left. + \dot{x}(0)\sin\left[t + \frac{3\lambda t}{4}H_0\right] + \sin\left[t + \frac{3\lambda t}{4}H_0\right]\dot{x}(0)\right]. \end{aligned} \tag{24}$$

This exactly coincides with the solutions given in [14, 15] and [19] and gives the correct classical frequency shift [23] in the limit $x(0) = a, \dot{x}(0) = 0$. Similarly we have

$$\begin{aligned} x(t)|_{m=6} = {} & \frac{1}{2\cos(\frac{5\lambda t}{4}n)}\left[x(0)\cos\left[t + \frac{5\lambda}{4}\left(H_0^2 + \frac{1}{4}\right)t\right] + \cos\left[t + \frac{5\lambda}{4}\left(H_0^2 + \frac{1}{4}\right)t\right]x(0)\right. \\ & \left. + \dot{x}(0)\sin\left[t + \frac{5\lambda}{4}\left(H_0^2 + \frac{1}{4}\right)t\right] + \sin\left[t + \frac{5\lambda}{4}\left(H_0^2 + \frac{1}{4}\right)t\right]\dot{x}(0)\right] \end{aligned} \tag{25}$$

$$\begin{aligned} x(t)|_{m=8} = {} & \frac{1}{2\cos[\frac{35\lambda}{64}(6n^2 + 3)t]}\left[x(0)\cos\left[t + \frac{35\lambda}{64}(4H_0^3 + 5H_0)t\right]\right. \\ & + \cos\left[t + \frac{35\lambda}{64}(4H_0^3 + 5H_0)t\right]x(0) + \dot{x}(0)\sin\left[t + \frac{35\lambda}{64}(4H_0^3 + 5H_0)t\right] \\ & \left. + \sin\left[t + \frac{35\lambda}{64}(4H_0^3 + 5H_0)t\right]\dot{x}(0)\right] \end{aligned} \tag{26}$$

and

$$\begin{aligned} x(t)|_{m=10} = {} & \frac{1}{2\cos[\frac{63\lambda t}{8}(n^3 + 2n)]}\left[x(0)\cos\left[t + \frac{63\lambda}{16}\left(H_0^4 + \frac{7}{2}H_0^2 + \frac{9}{16}\right)t\right]\right. \\ & + \cos\left[t + \frac{63\lambda}{16}\left(H_0^4 + \frac{7}{2}H_0^2 + \frac{9}{16}\right)t\right]x(0) \\ & + \dot{x}(0)\sin\left[t + \frac{63\lambda}{16}\left(H_0^4 + \frac{7}{2}H_0^2 + \frac{9}{16}\right)t\right] \\ & \left. + \sin\left[t + \frac{35\lambda}{64}\frac{63\lambda}{16}\left(H_0^4 + \frac{7}{2}H_0^2 + \frac{9}{16}\right)t\right]\dot{x}(0)\right]. \end{aligned} \tag{27}$$

The solutions for sextic and octic oscillators exactly coincide with the solution we obtained using the Taylor series approach [20] and all the solutions give the correct classical frequency shifts in the appropriate limit [24, 25].

## 5. Summary and concluding remarks

We conclude by noting that depending on the nature of nonlinearity in a physical problem the treatment of higher AHOs assumes significance, but studies in such oscillators (for $m > 4$) are not undertaken in the Heisenberg approach, presumably because the existing methods tend to introduce inordinate mathematical complications in a detailed study. In the present work we contemplate circumventing them by proving a theorem for the expansion of $(a^\dagger + a)^m_{\rm N}$. Thus the results of the present work are expected to serve a useful purpose for physicists working in nonlinear mechanics, molecular physics, quantum optics and quantum field theory.

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