An approach to quantum anharmonic oscillators via Lie algebra

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Abstract. We present a new Lie algebraic method to study the eigenvalues and eigenfunctions of quantum anharmonic oscillators. We consider the Hamiltonians for the simple harmonic and anharmonic oscillator as the two generators of a Lie algebra, whose other generators may be found exactly or up to any order of the parameter involved. Specifically, the closed commutator algebra for the quartic anharmonic oscillator is established in a perturbation sense. An element of this Lie group, turning out to be the four-photon operator, transforms the quartic anharmonic oscillator Hamiltonian to the harmonic one in a perturbation sense; thus, facilitating the calculation of the eigenvalues and eigenfunctions of the former.

1. Introduction
Simple harmonic oscillator is an idealized model to describe many phenomena in physics and chemistry. Anharmonic oscillator is a deviation from this idealized model to a realistic one. Rayleigh-Schrödinger perturbation theory has been widely used, providing the energy of an anharmonic oscillator, as a formal power series of the perturbation parameter involved [1, 2, 3, 4]. However, the power series diverges even for small coupling constants; thus, appropriate techniques must be applied to alleviate this problem [5, 6, 7, 8, 9, 10, 11, 12]. Several alternative approaches have also been developed; among them, a Lie algebraic method using canonical transformations [13], multiple scale method [14, 15, 16], quasilinearization method [17, 18], a variational method based on the squeezed states [19, 20] and Naundorf method [21] are mentioned.

In this work, we use a Lie algebra method to relate the Hamiltonian of an anharmonic oscillator to that of a harmonic one, in a perturbation sense. This is achieved via a canonical transformation, which is unique to the structure of the specific Hamiltonian under study. We introduce our method in section 2, where we apply it to two prototype trivial examples: a harmonic oscillator with a linear perturbation term and one with a quadratic perturbation term that just brings about a frequency shift. In section 3, a unitary transformation is found that relates the Hamiltonian of a quartic anharmonic oscillator to that of a harmonic one. It is observed that the matrix representation of the transformed Hamiltonian is diagonal, up to the first order in the perturbation parameter involved. The eigenvalues of the anharmonic oscillator are evaluated and the results are compared with those obtained from Rayleigh-Schrödinger perturbation theory. Finally, we deal with the discussion and conclusions in section 4.
2. Our Lie algebra method

The anharmonic oscillator, described by the Hamiltonian

\[ H_n = H_0 + \lambda x^n = \frac{p^2}{2} + \frac{x^2}{2} + \lambda x^n, \]  

(1)

is a deviation from the harmonic one, described by the Hamiltonian \( H_0 \). If \( N \) hermitian generators \( L_i \), including \( L_1 = H_0 \) and \( L_2 = H_n \), satisfying

\[ [L_i, L_j] = \sum_k c_{ij}^k L_k, \]  

(2)

form a closed commutator algebra, the operators \( L_i \) specify a Lie group, whose generators they are. The elements of this group are given by

\[ U = \exp(-i \sum_{i=1}^{N} \alpha_i L_i), \]  

(3)

where \( \alpha_i \)'s are real parameters. Now, an element of the group may be found that transforms \( H_0 \) to \( H_n \). This coming about, the eigenvalues and the eigenfunctions of the anharmonic oscillator can be obtained in terms of those of a harmonic one in a simple manner.

Now, let’s assume \( n = 1 \) in equation (1); we have

\[ H_1 = \frac{p^2}{2} + \frac{x^2}{2} + \lambda x = a^\dagger a + \frac{1}{2} + \lambda \left( a + a^\dagger \right), \]  

(4)

which may be considered as a harmonic oscillator in an external electric field. \( a \) and \( a^\dagger \) are the ordinary annihilation and creation operators. Considering the commutator \( [H_0, H_1] = \lambda (a^\dagger - a) / \sqrt{2} \), we realize that the operators \( H_0, H_1, i(a^\dagger - a) \) and the identity operator \( I \) form a closed commutator algebra and are the generators of a Lie group. The Glauber operator \( U_1 = \exp(a a^\dagger - a^\dagger a) \), with \( \alpha \) assumed real in this section, is an element of this group. The transformation of \( H_0 \) to \( H_1 \) is carried out in the following manner

\[ H_1 = U_1^\dagger H_0 U_1 - \frac{\lambda^2}{2}, \]  

(5)

where, \( \alpha \) has been replaced by \( \lambda / \sqrt{2} \) in \( U_1 \). Using (5) we find

\[ H_1 |U_1^\dagger n_a\rangle = \left[ (n + \frac{1}{2}) - \frac{\lambda^2}{2} \right] |U_1^\dagger n_a\rangle, \]

where \( \{|n_a\} \) are a-mode number states; meaning that the eigenvalues of \( H_1 \) are given by

\[ E_n = (n + \frac{1}{2}) - \frac{\lambda^2}{2}, \]  

(6)

and the eigenfunctions, called the displaced number states [22] are expressed by

\[ U_1^\dagger |n_a\rangle = e^{\frac{\lambda^2}{2} (a - a^\dagger)} |n_a\rangle. \]  

(7)

Now, we consider our second prototype trivial example. The Hamiltonian of a shifted-frequency harmonic oscillator, the case \( n = 2 \) in equation (1), is given by

\[ H_2 = \frac{p^2}{2} + \frac{x^2}{2} + \lambda x^2 = a^\dagger a + \frac{1}{2} + \lambda \left( a + a^\dagger \right)^2. \]  

(8)
In this case, we have \([H_0, H_2] = \lambda(a^{12} - a^2)\); therefore, the Hermitian operators \(H_0, H_2, i(a^{12} - a^2)\) and \(I\), form a closed commutator algebra and are the generators of a Lie group. The squeezing operator \(U_2 = \exp(\beta a^{12} - \beta^* a^2)\), with \(\beta\) assumed real, is an element of this group. The transformation of the fundamental mode operators \(a\) and \(a^{\dagger}\) into the new ones, \(b\) and \(b^{\dagger}\) under \(U_2\), is carried out by the following Bogoliubov transformations

\[
\begin{align*}
b &= U_2^\dagger a U_2 = \mu a + \nu a^{\dagger}, \\
b^{\dagger} &= U_2^\dagger a^{\dagger} U_2 = \mu a^{\dagger} + \nu a,
\end{align*}
\]

where, \(\mu = \cosh(2\beta)\) and \(\nu = \sinh(2\beta)\). As \(\mu^2 - \nu^2 = 1\), we have also \([b, b^{\dagger}] = 1\). The transformed Hamiltonian under \(U_2\) is given by

\[
H_2 = \sqrt{1 + 2\lambda \mu} U_2^\dagger H_0 U_2 = \sqrt{1 + 2\lambda} (b^{\dagger} b + \frac{1}{2}),
\]

where, \(\lambda = 2\mu\nu/(\mu - \nu)^2\) has been assumed. Using equation (9) we find

\[
H_2[U_2^\dagger |n\rangle_a] = \sqrt{1 + 2\lambda(n + \frac{1}{2})} |U_2^\dagger n\rangle_a,
\]

or

\[
H_2 |n\rangle_b = \sqrt{1 + 2\lambda(n + \frac{1}{2})} |n\rangle_b,
\]

implying that eigenfunctions of the shifted-frequency harmonic oscillator, the \(b\)-mode number states, or squeezed number states \([22]\), are given by \(|n\rangle_b = U_2^\dagger |n\rangle_a\), and the corresponding energies by \(\sqrt{1 + 2\lambda(n + \frac{1}{2})}\).

3. Quartic anharmonic oscillator

Now we consider the quartic anharmonic oscillator. Its Hamiltonian in terms of the fundamental mode operators \(a\) and \(a^{\dagger}\), may be given by

\[
H_4 = a^{\dagger} a + \frac{1}{2} + \lambda \left(\frac{a + a^{\dagger}}{\sqrt{2}}\right)^4.
\]

We can show that

\[
[H_0, H_4] = -iL_3 - 3iL_4 - 2iL_5,
\]

where,

\[
L_3 = i\lambda(a^{14} - a^4), \\
L_4 = i\lambda(a^{12} - a^2), \\
L_5 = i\lambda(a^{13}a - a^4 a^{\dagger}).
\]

Inspecting the mutual commutators between the operators \(H_0, H_4, L_3, L_4\) and \(L_5\), we are finally led to prove that \(H_0, H_4, i\lambda(a^{14} - a^4), i\lambda(a^{12} - a^2), i\lambda(a^{13}a - a^4 a^{\dagger}), \lambda(a^{14} + a^4), \lambda(a^{12} + a^2), \lambda(a^{13}a - a^4 a^{\dagger})\) and \(I\) form a closed commutator algebra up to the first order, if the perturbation parameter \(\lambda\) is small, and therefore they are the generators of a Lie group, up to that order. We now focus on the following element of this group, known as the four photon operator \([23]\)

\[
U_4 = \exp[A\lambda(a^{14} - a^4) + B\lambda(a^{12} - a^2) + C\lambda(a^{13}a - a^4 a^{\dagger})],
\]

3
where $A$, $B$ and $C$ are real parameters. This operator transforms the fundamental mode operators, $a$ and $a^\dagger$ to the new ones $c$ and $c^\dagger$. Using Baker-Campbell-Hausdorff relation up to the first order, they may be expressed by the following expressions

$$c = U_4^\dagger a U_4 = a + \lambda (4Aa^3 + 2Ba^2 + 3Ca^2 a - Ca^3),$$

$$c^\dagger = U_4^\dagger a^\dagger U_4 = a^\dagger + \lambda (4Aa^3 + 2Ba^2 + 3Ca^2 a^2 - Ca^3).$$

(13) 

(14)

It should be emphasized that $c$ and $c^\dagger$ also obey the canonical commutation relation $[c, c^\dagger] = 1$; therefore, we have introduced a new class of Bogoliubov transformations by (13) and (14). Assuming $A = 1/16$, $B = 3/4$ and $C = 1/2$, the four photon operator transforms $H_0$ to $H_4$, up to the first order in the parameter $\lambda$, as follows

$$U_4^\dagger H_0 U_4 = c^\dagger c + \frac{1}{2} = H_4 - \frac{3\lambda}{2} (N_a^2 + N_a) - \frac{3\lambda}{4},$$

$$H_0 = U_4 H_4 U_4^\dagger - \frac{3\lambda}{2} N_a (N_a + 1) - \frac{3\lambda}{4},$$

(15)

where, $N_a = a^\dagger a$ is the normal number operator. Using equation (15), we find

$$H_4[U_4^\dagger |n\rangle_a] = |n + \frac{1}{2} + \frac{3\lambda}{4} + \frac{3\lambda}{2} n(n+1)||U_4^\dagger |n\rangle_a].$$

Thus, the eigenstates of the quartic anharmonic oscillator, our $c$-mode number states, are given by

$$|n\rangle_c \equiv U_4^\dagger |n\rangle_a = e^{-\lambda/4} (a^4 - a^3 + \frac{1}{4} (a^2 - a^2) + \frac{1}{2} (a^2 a - a^3 a)) |n\rangle_a,$$

(16)

and the first order perturbed energies are expressed by

$$E_n = n + \frac{1}{2} + \frac{3\lambda}{4} + \frac{3\lambda}{2} n(n+1).$$

(17)

The above results are in complete agreement with those obtained, using first order Rayleigh-Schrödinger perturbation theory [24].

Furthermore, although (16) and (17) are formally derived up to first order in the parameter $\lambda$, it is worthwhile to investigate the contribution of higher order terms to the energy using (16). For example, we calculate the expectation value of $H_4$ in the $c$-mode number states basis up to the fourth order; we find

$$E_0 = 0.5 + 0.75\lambda - 2.625\lambda^2 + 20.8125\lambda^3 - 104.098\lambda^4 + \ldots,$$

(18)

Bender and Wu also give the following perturbation series, for the ground state energy $E_{0,B}$, of the quartic anharmonic oscillator which we write down up to the fourth order also [1]

$$E_{0,B} = 0.5 + 0.75\lambda - 2.625\lambda^2 + 20.8125\lambda^3 - 241.289\lambda^4 + \ldots.$$ 

(19)

We note that the result (18) agrees with (19), up to the third order in the parameter $\lambda$. We have also ascertained that our result (18) is in agreement, up to the third order in the parameter $\lambda$, with those obtained from multiple scale method [16], and also those from Rayleigh-Schrödinger perturbation theory [24].

The agreement between (18) and (19) should not surprise the reader. We should remember that this situation is similar to the one we encounter in Rayleigh - Schrödinger perturbation theory. Moreover, both series are divergent even for small values of $\lambda$, and one has to truncate the series, to get any physical result. Obviously, a judicious choice of the truncation order is essential to the finding of good results [12]. For example, using (18) we calculate the ground state energy up to the fourth order; for $\lambda = 0.1$ we find $E_0 = 0.5591527$. Comparing this result with the exact value $E_0 = 0.559146327183519576$ obtained by Vinette and Čížek [25], the error is about 0.001 percent.
4. Discussion
We have introduced a concise method to study anharmonic oscillators. It is based on the construction of a Lie group, whose generators include $H_0$ and $H_n$. The generator of the group $H_0$ may be transformed to the generator $H_n$ by a unitary transformation, endowed by an element of the group. If a closed commutator algebra is formed exactly, the method can be used to obtain exact eigenvalues and eigenfunctions of $H_n$. However, the commutator algebra is generally obeyed up to some order of the parameter $\lambda$, thus the eigenvalues and eigenfunctions of $H_n$ are found approximately. We applied the method to obtain the energy eigenvalues of a quartic anharmonic oscillator; the results are in agreement with the other methods, up to third order in the parameter $\lambda$.

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