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Research Article

A Closed Form Solution for Quantum Oscillator Perturbations Using Lie Algebras

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Abstract We give a new solution to a well-known problem, that of computing perturbed eigenvalues for quantum oscillators. This article is nearly self contained and begins with all the necessary algebraic tools to make the subsequent calculations. We define a new family of Lie algebras relevant to making computations for perturbed (anharmonic) oscillators, and show that the only two formally closed solutions are indeed harmonic oscillators themselves. Through elementary combinatorics and noncanonical forms of well-known Lie algebras, we are able to obtain a fully closed form solution for perturbed eigenvalues to first order.

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1 Introduction

The goal of the present paper is primarily to exhibit the effectiveness of using Lie algebras to compute exact perturbation eigenvalues for quantum anharmonic oscillators in one dimension. There are, however, several goals secondary in stature, but which merit discussion. The first of these is to enable the reader to work with Weyl algebras in the abstract. Two presentations of it arise readily in quantum physics. In particular, the first is the algebra of position and momentum operators in nonrelativistic mechanics wherein $[x,p] = i\hbar$. The second is the algebra of ladder operators $[a,a^\dagger] = 1$. It is the second presentation with which we will be primarily concerned in this paper. Of course, the first presentation may be made to look like the second by considering not p, but instead the simple derivative $\frac{d}{dx}$ whereby one has $[\frac{d}{dx},x] = 1$.

The main result is for a Hamiltonian of the form

$$H_{2k} = \frac{1}{2}\left(x^2 - \frac{d^2}{dx^2}\right) + \lambda x^{2k}.$$

We have computed the first-order perturbation of its eigenvalues as

$$E_n = n + \frac{1}{2} + \frac{\lambda}{2^k}\left(\sum_{j=0}^{k} j! \begin{Bmatrix} 2k \\ k \end{Bmatrix}_{k-j} \binom{n}{j}\right),$$

where E_n is the nth energy level and $\left\{ {\ell \atop m} \right\}_k$ is a Weyl binomial coefficient.

In Section 2, we give a brief outline of the algebraic and combinatorial techniques necessary to make all relevant computations obtained in this article. This includes normal ordering or Weyl variables, polynomials of Weyl variables, Baker-Campbell-Hausdorff formula and Hadamard lemma, as well as basic combinatorial structures in Weyl variables. Section 3 gives a concise description of the method of Jafarpour and Ashfar. The original paper is brief and focuses more on numerical computations and advantages to this method. Here, we define our Lie algebras up to any finite order. In section 4 the focus shifts directly to Lie algebras of order one in λ and computes their dimensions. It should be noted that all of these Lie algebras have a central element. Section 5 gets to the heart of the matter, giving a closed form solution to perturbed quantum oscillators in one dimension. While it has been known for several decades that the first-order perturbation of an odd potential is zero, no closed form solution for even potentials has been given. Using our Lie algebras up to order one in λ, we are finally able to give such a solution up to order one. Furthermore, the perturbed ground state is given exactly for any potential given by an analytic function. Section 6 extends the range of this method. With substantially more time, we may compute closed form solutions up to order n in λ. Furthermore, this method may be used to obtain exact solutions for harmonic oscillators in higher dimensions, including magnetic fields, or with dynamic coupling.

2 Algebraic preliminaries

2.1 Normal ordering and Weyl binomial coefficients

For any abstract Weyl algebra determined by two elements A and B obeying $[A, B] = 1$, an ordering of a polynomial in A and B will be said to be *normally ordered* if all powers of B appear to the left of powers of A. For example A^3B^2 is not normally ordered, but B^2A^3 is. In our case $a^\dagger$ will always be placed to the left of a. As it is well known in elementary quantum mechanics, one may move back and forth between presentations of problems in position-momentum coordinates and annihilator-creator coordinates with the following equivalences:

$$x = \frac{a + a^\dagger}{\sqrt{2}}, \quad p = \frac{a - a^\dagger}{i\sqrt{2}}. \tag{2.1}$$

Since this paper is concerned with anharmonic oscillators, we will be concerned with x^n in the potential. Thus, we need an efficient way of normally ordering $(a + a^\dagger)^n$.

Lemma 1. *Let A and B determine a Weyl algebra so that $[A, B] = 1$. The normal ordering of $(A + B)^n$ is given by*

$$(A + B)^n = \sum_{m=0}^{n} \sum_{k=0}^{\min\{m,n-m\}} \begin{Bmatrix} n \\ m \end{Bmatrix}_k B^{m-k}A^{n-m-k}, \tag{2.2}$$

where

$$\begin{Bmatrix} n \\ m \end{Bmatrix}_k = \frac{n!}{2^k k!(m-k)!(n-m-k)!} \tag{2.3}$$

is the Weyl binomial coefficient.

The proof of this lemma involves nothing more than counting commutations. A more combinatorial approach is undertaken in [3].

Example 2. We will use the fourth-order relation explicitly later, so here is an example of how the Weyl coefficients factor in:

$$(a + a^\dagger)^4 = a^{\dagger 4} + 4a^{\dagger 3}a + 6a^{\dagger 2}a^2 + 4a^\dagger a^3 + a^4 + 6a^{\dagger 2} + 12a^\dagger a + 6a^2 + 3.$$

Remark 3. Notice that

$$\begin{Bmatrix} n \\ m \end{Bmatrix}_k = \begin{Bmatrix} n \\ n-m \end{Bmatrix}_k.$$

If one wishes to attempt calculations within a Weyl algebra, it may be useful to compute with abstract elements A, B first and then plug into a specific situation one has in mind. One other useful tip is that if one has Weyl variables A, B, then it can be convenient to consider representing the algebra as $\frac{d}{dB}, B$ or $A, -\frac{d}{dA}$. This becomes consistent with the first presentation considered. For example, one peculiar formula which is arguably easier to compute with abstract Weyl variables is

$$\mu^{x\partial_x} f(x) = f(\mu x). \tag{2.4}$$

2.2 Baker-Campbell-Hausdorff and the Hadamard lemma

We will be concerned throughout much of this paper with exponentiating noncommuting variables. We run into a stopping block in trying to compute the exponentials explicitly. The main issue is that for noncommuting variables X, Y we see

$$e^Y e^X \neq e^{Y+X} = e^{X+Y} \neq e^X e^Y.$$

The *Baker-Campbell-Hausdorff* formula is the solution to $Z = \log(e^X e^Y)$. The explicit solution is formally given as symmetric sums and differences of nested commutators in X and Y. One may find this expression in nearly any textbook on advanced quantum mechanics. We will not be concerned, however, with isolated exponentials, but rather expressions of the form

$$e^X Y e^{-X}.$$

Using elementary combinatorics and the Baker-Campbell-Hausdorff formula, one can arrive at the *Hadamard lemma*.

Lemma 4. *Let X, Y be noncommuting variables, then one has*

$$e^X Y e^{-X} = Y + [X, Y] + \frac{1}{2!}[X, [X, Y]] + \frac{1}{3!}[X, [X, [X, Y]]] + \cdots . \tag{2.5}$$

If one allows the notation $[X^{(n)}, Y] = [X, [\ldots, [X, Y]]]$, then one may write more succinctly

$$e^X Y e^{-X} = \sum_{k=0}^{\infty} \frac{1}{k!}[X^{(k)}, Y]. \tag{2.6}$$

2.3 The formula often desired and rarely known

One final assertion about Weyl variables in the algebraic preliminaries must be the formula

$$[A^n, B^m] = \sum_{k=1}^{\min\{n,m\}} k! \binom{m}{k} \binom{n}{k} B^{m-k} A^{n-k}. \tag{2.7}$$

This formula is often left as an exercise in quantum mechanics texts and sometimes in homological algebra, but rarely is it completed. One might jokingly say it is similar to the snake lemma in that no one knows if it's really true since the only persons who have ever proven it are graduate students. All kidding aside, this is indeed the correct formula for normally ordering variables obeying the Weyl relation.

3 Using Lie algebras to determine perturbed eigenvalues

The main impetus for this research comes from the paper [2]. The goal of this section is to explicate in a reasonably clear manner the content of that paper.

The premise upon which [2] begins is the idea that we can create a new Lie algebra from simply taking commutators of the unperturbed Hamiltonian H_0 and the new anharmonic Hamiltonian H_n. For the sake of mathematical simplicity, the Hamiltonians in question are given as essentially unitless operators:

$$H_0 = \frac{1}{2}(p^2 + x^2) = a^\dagger a + \frac{1}{2}, \quad H_n = H_0 + \lambda x^n = a^\dagger a + \frac{1}{2} + \frac{\lambda}{\sqrt{2}^n}(a + a^\dagger)^n. \tag{3.1}$$

As one may infer, we have made the following assumptions and simplifications:

1. $\hbar = \omega = m = 1$,
2. $a = \frac{x+ip}{\sqrt{2}}, a^\dagger = \frac{x-ip}{\sqrt{2}}$,
3. $x = \frac{a+a^\dagger}{\sqrt{2}}, p = \frac{a^\dagger - a}{i\sqrt{2}}$.

Let us now give the formulation of the Lie algebras.

Definition 5. The Lie algebra $\mathcal{A}_n^{(k)} = \{L_m\}_{m \in I}$ is generated by the elements

$$L_1 = H_0, \quad L_2 = H_n$$

and other L_m satisfying

$$[L_i, L_j] = \sum c_{ijm} L_m, \tag{3.2}$$

for some structure constants $c_{ijm} \in \mathbb{C}$. Furthermore, this Lie algebra should be closed under commutators up to order λ^k. In other words, no L_m should be of the form $\lambda^{k+1}(a^{\dagger t} a^s - a^{\dagger s} a^t)$ for any s, t. That is, formally we require $\lambda^{k+1} = 0$ within the Lie algebra.

In the case of this paper, we will consider $\mathcal{A}_n^{(1)}$ unless otherwise explicitly stated. In fact, [2] only considers Lie algebras up to order one in λ with the exceptions of $n = 1$ and $n = 2$ because these determine harmonic oscillators and their solutions are already known. We deal with the special technique for solving harmonic oscillators in the appendix.

Once the algebra $\mathcal{A}_n^{(1)}$ is determined, we proceed in the following way. Suppose

$$[L_1, L_2] = \sum_{k=3}^{j} c_{12k} L_k \tag{3.3}$$

where each L_k is of the form

$$\lambda\big(a^{\dagger m} a^{\ell} - a^{\dagger \ell} a^{m}\big). \tag{3.4}$$

The symmetry of these L_k is important and comes back in an important way due to the normal ordering procedures we have adopted. We will see this explicitly in the computations.

We then construct a unitary element of the associated Lie group by

$$U = \exp\left(\sum_{k=3}^{j} \alpha_k L_k\right). \tag{3.5}$$

This says that the only L_k allowed in our unitary are those arising directly from the commutator $[L_1, L_2]$. The α_k are real constants which we will tune as necessary.

Once we produce such a unitary, we make a transformation from H_0 to H_n by

$$U^{\dagger} H_0 U = H_n - \Lambda_n. \tag{3.6}$$

In each case, Λ_n is an operator which simply controls the perturbations of eigenvalues. Furthermore, by the clever choice of U we will have $[U, \Lambda_n] = 0 + O(\lambda^2)$. Due to the Hadamard lemma we can produce Λ_n by computing simple commutators.

At this stage one may write the new eigenvectors as $U^{\dagger}|j\rangle$, where $|j\rangle$ are the eigenvectors for the harmonic Hamiltonian with eigenvalues $j + \frac{1}{2}$. Therefore, up to order λ^2 our equation now reads

$$\begin{aligned} H_n U^{\dagger}|j\rangle &= \big(U^{\dagger} H_0 U + \Lambda_n\big) U^{\dagger}|j\rangle = U^{\dagger} H_0 |j\rangle + \Lambda_n U^{\dagger}|j\rangle \\ &= U^{\dagger}\left(j + \frac{1}{2}\right)|j\rangle + U^{\dagger}\Lambda_n|j\rangle = \left(j + \frac{1}{2} + \lambda_n\right) U^{\dagger}|j\rangle. \end{aligned} \tag{3.7}$$

In essense, depending on the form of Λ_n, we will be able to read off the first-order perturbation eigenvalues (λ_n) of H_n with relative ease.

A natural question arises as to when we can solve this system explicitly. The work in [2] makes a passing statement which we will now state as a formal theorem.

Theorem 6. *If the Lie Algebra $\mathcal{A}_n$ is closed (in all orders of λ), then one can solve the nth order anharmonic oscillator in closed form.*

Proof. Let $\mathcal{A}_n = \{L_k\}_{k=1}^{N}$ be a closed Lie algebra corresponding to the Hamiltonian H_n. Then, consider the general Lie group element given by

$$U = \exp\left(\sum_{k=1}^{N} \alpha_k L_k\right) =: \exp(L).$$

From the Hadamard lemma, we obtain

$$U^{\dagger} H_0 U = \sum_{k=1}^{\infty} \frac{1}{k!}\big[L^{(k)}, H_0\big]. \tag{3.8}$$

Since $\mathcal{A}_n$ is closed, the commutators $[L^{(k)}, H_0]$ either vanish or give Lie algebra elements with some periodicity. In this way, we can formally sum them in a power series. Setting our parameters to appropriate values, we obtain

$$U^{\dagger} H_0 U = H_n + \text{perturbations}.$$ □

Remark 7. It should be noted, however, that whenever $n > 2$, $\mathcal{A}_n$ is known to be infinite dimensional. Therefore, the only truly closed Lie algebras are $\mathcal{A}_1$ and $\mathcal{A}_2$. The solutions to the corresponding Hamiltonians are known exactly, as these are shifted harmonic oscillators.

It is also of some considerable interest to note that both $\mathcal{A}_1$ and $\mathcal{A}_2$ are four-dimensional closed Lie algebras with center. Therefore, they are each isomorphic to $\mathfrak{gl}_2$ albeit noncanonically.

4 Lie algebras up to order one in λ

We begin the computation of the Lie algebras by giving an important commutator relation:

$$\left[a^\dagger a, a^{\dagger k}a^\ell \pm a^{\dagger \ell}a^k\right] = (k-\ell)\left(a^{\dagger k}a^\ell \mp a^{\dagger \ell}a^k\right). \tag{4.1}$$

This equation paired with the symmetry of Weyl binomial coefficients points us to assigning $a^{\dagger n}a^m - a^{\dagger m}a^n$ as our Lie algebra elements. Let us begin by computing $[H_0, H_n]$:

$$\begin{aligned}\left[H_0, H_n\right] &= \left[H_0, H_0 + \frac{\lambda}{\sqrt{2}^n}\left(a^\dagger + a\right)^n\right] = \left[H_0, \frac{\lambda}{\sqrt{2}^n}\left(a^\dagger + a\right)^n\right] = \frac{\lambda}{\sqrt{2}^n}\left[a^\dagger a, \left(a^\dagger + a\right)^n\right] \\ &= \frac{\lambda}{\sqrt{2}^n}\left[a^\dagger a, \sum_{k,m}\left\{ {n \atop m} \right\}_k \left(a^{\dagger m-k}a^{n-m-k} + a^{\dagger n-m-k}a^{m-k}\right)\right] \\ &= \frac{\lambda}{\sqrt{2}^n}\sum_{k,m}\left\{ {n \atop m} \right\}_k (2m-n)\left(a^{\dagger m-k}a^{n-m-k} - a^{\dagger n-m-k}a^{m-k}\right).\end{aligned} \tag{4.2}$$

We will throw away the multiplicative constants in favor of rescaling them by α_k in our general Lie group element. Therefore, the first batch of elements revealed to us are those of the form $\lambda(a^{\dagger\ell}a^m - a^{\dagger m}a^\ell)$. Once we realize these, we begin commuting again with H_0 to find more elements of the form $\lambda(a^{\dagger\ell}a^m + a^{\dagger m}a^\ell)$. In order to close $\mathcal{A}_n^{(1)}$ we also need to add a central element I to our Lie algebra. All other commutators will involve terms with λ^2 and therefore we disregard them in $\mathcal{A}_n^{(1)}$.

Remark 8. Notice that no elements of the form $a^{\dagger n}a^n$ appear anywhere. This is because they can be written in terms of the number operator $N = a^\dagger a$ which commutes with H_0.

Given a general Hamiltonian H_n, with special exceptions, by simple combinatorial formulae one infers the number of generators for $\mathcal{A}_n^{(1)}$ by

$$\left|\mathcal{A}_{2k}^{(1)}\right| = (k+1)k + 3, \quad \left|\mathcal{A}_{2k+1}^{(1)}\right| = (k+1)k + 3. \tag{4.3}$$

Example 9. Let us take a quick look at $\mathcal{A}_6^{(1)}$. Of course, we let $L_1 = H_0$ and $L_2 = H_6$. By our computation, we know the generators arising from $[L_1, L_2]$ are as follows:

$$\lambda\left(a^{\dagger 6} - a^6\right),\ \lambda\left(a^{\dagger 5}a - a^\dagger a^5\right),\ \lambda\left(a^{\dagger 4}a^2 - a^{\dagger 2}a^4\right),\ \lambda\left(a^{\dagger 4} - a^4\right),\ \lambda\left(a^{\dagger 3}a - a^\dagger a^3\right),\ \lambda\left(a^{\dagger 2} - a^2\right).$$

Furthermore, commuting these with L_1 we obtain similarly symmetric elements with plus signs. Finally, we add in I to account for commuting elements. Notice that if we commute any other elements, we obtain an element in $\mathcal{A}_6^{(2)}$ which we have formally disallowed for now. Therefore, $|\mathcal{A}_6^{(1)}| = 15 = (3+1)3 + 3$ as previously stated.

5 Explicit computations

In this section, we will derive the first-order perturbation for all anharmonic oscillators with Hamiltonians of the form

$$H_n = \frac{1}{2}\left(p^2 + x^2\right) + \lambda x^n.$$

There are two distinct cases for computing first-order perturbations; odd and even. We will treat the odd case first.

For the sake of uniformity in our calculations, we will consider Hamiltonians of the form H_{2k-1} and H_{2k}.

5.1 Odd powered potentials

From our earlier computations of $[H_0, H_{2k-1}]$ and our prescribed form of U, we have

$$U = \exp\left(\lambda \sum_{\ell=0}^{m-1} \sum_{m=1}^{k} \alpha_{m,\ell} a^{\dagger 2m-1-\ell} a^{\ell} - a^{\dagger \ell} a^{2m-1-\ell}\right). \tag{5.1}$$

By requiring $\alpha_{m,\ell} \in \mathbb{R}$, we obtain $U^\dagger = U^{-1}$ and we may now apply the Hadamard lemma. Letting

$$X := \lambda \sum_{\ell=0}^{m-1} \sum_{m=1}^{k} \alpha_{m,\ell} \big(a^{\dagger 2m-1-\ell} a^{\ell} - a^{\dagger \ell} a^{2m-1-\ell}\big)$$

we have

$$U^\dagger H_0 U = H_0 + \big[-X, H_0\big] + \frac{1}{2!}\big[-X, \big[-X, H_0\big]\big] + \cdots . \tag{5.2}$$

We notice immediately that X contains a multiplicative factor of λ and since we have $\lambda^2 = 0$ we may ignore all terms past $[-X, H_0]$.

Using previous computations and elementary properties of derivations we have

$$\big[H_0, X\big] = \lambda \sum_{\ell=0}^{m-1} \sum_{m=1}^{k} \alpha_{m,\ell}(2m-1-2\ell)\big(a^{\dagger 2m-1-\ell} a^{\ell} + a^{\dagger \ell} a^{2m-1-\ell}\big). \tag{5.3}$$

If we recognize that

$$x^{2k-1} = \frac{(a+a^\dagger)^{2k-1}}{\sqrt{2}^{2k-1}} = \frac{1}{\sqrt{2}^{2k-1}} \sum_{m=0}^{2k-1} \sum_{j=0}^{\min\{m,2k-1-m\}} \begin{Bmatrix} 2k-1 \\ m \end{Bmatrix}_j a^{\dagger m-j} a^{2k-1-m-j}, \tag{5.4}$$

we see that in order to produce $H_{2k-1} = H_0 + \lambda x^{2k-1}$ we need to set

$$\alpha_{m,\ell}(2m-2\ell-1) = \frac{1}{\sqrt{2}^{2k-1}} \begin{Bmatrix} 2k-1 \\ k-m+\ell \end{Bmatrix}_{k-m}. \tag{5.5}$$

Notice what we have done. We have transformed H_0 into $H_{2k-1} + O(\lambda^2)$. Hence, there is no perturbation term up to first order.

Example 10. Let us compute the example of $H_1 = H_0 + \lambda x$ explicitly. We already know that this is a shifted harmonic oscillator, where a simple change of variables reveals that the energy eigenvalues are $n + \frac{1}{2} - \frac{\lambda^2}{2}$.

In our case the Lie algebra simplifies slightly and is fully closed as

$$H_0, H_1, \lambda(a^\dagger - a), I.$$

Our appropriate unitary transformation U is therefore given as

$$U = \exp\big(\alpha\lambda(a^\dagger - a)\big).$$

We can compute this even more explicitly than before given that $[a^\dagger - a, a^\dagger] = [a^\dagger - a, a] = -1$. In this case, we know

$$[A, B] = \beta \in \mathbb{C} \Longrightarrow \big[A, e^B\big] = \beta e^B \tag{5.6}$$

for any abstract operators A, B.

Therefore $[a, U] = \alpha\lambda U$ and $[a^\dagger, U] = \alpha\lambda U$,

$$\begin{aligned} U^\dagger H_0 U &= U^\dagger a^\dagger a U + \frac{1}{2} = U^\dagger a^\dagger U(\alpha\lambda + a) + \frac{1}{2} = U^\dagger U(a^\dagger + \alpha\lambda)(a + \alpha\lambda) + \frac{1}{2} \\ &= a^\dagger a + \frac{1}{2} + \alpha\lambda(a^\dagger + a) + \alpha^2\lambda^2. \end{aligned}$$

Setting $\alpha = \frac{1}{\sqrt{2}}$ we derive

$$U^\dagger H_0 U = H_1 + \frac{\lambda^2}{2}. \tag{5.7}$$

This is exactly the result we previously knew. Notice, however, that there is no λ term. The first perturbation term is order λ^2.

Example 11. To better see the odd powered result more explicitly, let us compute the result for H_5. Our Lie algebra up to order one is given by

$$\begin{aligned}&\lambda(a^{\dagger 5}-a^5),\ \lambda(a^{\dagger 4}a-a^{\dagger}a^4),\ \lambda(a^{\dagger 3}a^2-a^{\dagger 2}a^3),\ \lambda(a^{\dagger 3}-a^3),\ \lambda(a^{\dagger 2}a-a^{\dagger}a^2),\ \lambda(a^{\dagger}-a),\\&\lambda(a^{\dagger 5}+a^5),\ \lambda(a^{\dagger 4}a+a^{\dagger}a^4),\ \lambda(a^{\dagger 3}a^2+a^{\dagger 2}a^3),\ \lambda(a^{\dagger 3}+a^3),\ \lambda(a^{\dagger 2}a+a^{\dagger}a^2),\ \lambda(a^{\dagger}+a),\\&H_0,\ H_5,\ I.\end{aligned}$$

Therefore U is

$$U=\exp\left(\lambda\left(\alpha_{3,0}(a^{\dagger 5}-a^5)+\alpha_{3,1}(a^{\dagger 4}a-a^{\dagger}a^4)+\cdots+\alpha_{1,0}(a^{\dagger}-a)\right)\right).$$

Our Hamiltonian transforms as

$$\begin{aligned}U^{\dagger}H_0U&=H_0+\lambda\big[H_0,\alpha_{3,0}(a^{\dagger 5}-a^5)+\alpha_{3,1}(a^{\dagger 4}a-a^{\dagger}a^4)+\cdots+\alpha_{1,0}(a^{\dagger}-a)\big]+O(\lambda^2)\\&=H_0+\lambda\big(5\alpha_{3,0}(a^{\dagger 5}+a^5)+3\alpha_{3,1}(a^{\dagger 4}a+a^{\dagger}a^4)+\cdots+\alpha_{1,0}(a^{\dagger}+a)\big).\end{aligned}$$

Setting

$$\begin{aligned}&\alpha_{3,0}=2^{-5/2}/5,&&\alpha_{3,1}=2^{-5/2}5/3,&&\alpha_{3,2}=2^{-5/2}10,\\&\alpha_{2,0}=2^{-5/2}10/3,&&\alpha_{2,1}=2^{-5/2}30,&&\alpha_{1,0}=2^{-5/2}15,\end{aligned}$$

we obtain

$$U^{\dagger}H_0U=H_0+\lambda x^5+O(\lambda^2)=H_5+O(\lambda^2). \tag{5.8}$$

5.2 Even powered potentials

It is the goal of this section to show that the first-order perturbation energies for oscillators corresponding to H_{2k} are

$$n+\frac{1}{2}+\frac{\lambda}{2^k}\left(\sum_{j=0}^{k}j!\begin{Bmatrix}2k\\k\end{Bmatrix}_{k-j}\binom{n}{j}\right). \tag{5.9}$$

This result is obtained rather easily utilizing the technology we have developed for odd powered potentials. We only need to realize that the operators which are not Lie algebra elements are of the form $a^{\dagger n}a^n$. This comes from the required symmetry of our generators. Hence our unitary U will appear exactly as in the odd powered case and the Hadamard lemma yields

$$U^{\dagger}H_0U=H_0+\lambda x^{2k}-\frac{\lambda}{2^k}\sum_{j=0}^{k}\begin{Bmatrix}2k\\k\end{Bmatrix}_{k-j}a^{\dagger j}a^j+O(\lambda^2). \tag{5.10}$$

The only thing left to pretty up our example is changing $a^{\dagger k}a^k$ into an expression of number operators.

Recall that $N=a^{\dagger}a$ has nonnegative integer eigenvalues given by $N|n\rangle=n|n\rangle$. In this way, any expression $f(N)$ in our perturbation expansion will give eigenvalues $f(n)$ by the functional calculus.

Proposition 12.

$$a^{\dagger k}a^k=k!\binom{N}{k}. \tag{5.11}$$

Proof. We refer back to our commutation relation $[A^n,B^m]$ from Section 2.3. Thus we have

$$\begin{aligned}a^{\dagger k}a^k&=a^{\dagger}(a^{\dagger k-1}a)a^{k-1}=a^{\dagger}(aa^{\dagger k-1}-(k-1)a^{\dagger k-2})a^{k-1}\\&=(a^{\dagger}a)a^{\dagger k-1}a^{k-1}-(k-1)a^{\dagger k-1}a^{k-1}\\&=(N-(k-1))a^{\dagger k-1}a^{k-1}.\end{aligned}$$

Repeating this we see that

$$a^{\dagger k}a^k=N(N-1)\cdots\big(N-(k-1)\big)=k!\binom{N}{k}. \tag{5.12}$$

□

It is merely a matter of rearranging terms to see that

$$U^\dagger H_0 U = H_{2k} - \frac{\lambda}{2^k}\sum_{j=0}^{k} j! \left\{ \begin{matrix} 2k \\ k \end{matrix} \right\}_{k-j} \binom{N}{j} + O(\lambda^2). \tag{5.13}$$

Example 13. Let us look briefly at the Hamiltonian

$$H_4 = a^\dagger a + \frac{1}{2} + \frac{\lambda}{4}(a^\dagger + a)^4.$$

This is the famous quartic which has received much attention in texts and papers. We can check our results against those of standard perturbation theory.

Our Lie algebra $\mathcal{A}_4^{(1)}$ is given by

$$\lambda(a^{\dagger 4} - a^4),\ \lambda(a^{\dagger 3}a - a^\dagger a^3),\ \lambda(a^{\dagger 2} - a^2),\ \lambda(a^{\dagger 4} + a^4),\ \lambda(a^{\dagger 3}a + a^\dagger a^3),\ \lambda(a^{\dagger 2} + a^2),\ H_0,\ H_4,\ I.$$

Our unitary is given by

$$U = \exp\left(\lambda(\alpha_{2,0}(a^{\dagger 4} - a^4) + \alpha_{2,1}(a^{\dagger 3}a - a^\dagger a^3) + \alpha_{1,0}(a^{\dagger 2} - a^2))\right).$$

From here we must simply crank the handle for our machine and we realize that

$$\begin{aligned} U^\dagger H_0 U &= H_0 + \left[H_0, \lambda(\alpha_{2,0}(a^{\dagger 4} - a^4) + \alpha_{2,1}(a^{\dagger 3}a - a^\dagger a^3) + \alpha_{1,0}(a^{\dagger 2} - a^2))\right] \\ &= H_0 + \lambda(4\alpha_{2,0}(a^{\dagger 4} + a^4) + 2\alpha_{2,1}(a^{\dagger 3}a + a^\dagger a^3) + \alpha_{1,0}(a^{\dagger 2} + a^2)). \end{aligned} \tag{5.14}$$

Setting

$$\alpha_{2,0} = 1/16, \quad \alpha_{2,1} = 1/2, \quad \alpha_{1,0} = 3/4,$$

we arrive at

$$U^\dagger H_0 U = H_4 - \frac{\lambda}{4}(6a^{\dagger 2}a^2 + 12a^\dagger a + 3) = H_4 - \frac{3\lambda}{2}(N(N+1)) - \frac{3\lambda}{4}. \tag{5.15}$$

If we look to the ground state, we see that

$$E_0 = \frac{1}{2} + \frac{3\lambda}{4} + O(\lambda^2)$$

which agrees with the standard perturbation theory.

In particular, the perturbed ground state of the anharmonic oscillator corresponding to H_{2k} is given by

$$E_0 = \frac{1}{2} + \frac{\lambda}{2^k}\left\{ \begin{matrix} 2k \\ k \end{matrix} \right\}_k + O(\lambda^2) = \frac{1}{2} + \frac{\lambda(2k)!}{2^{2k}k!} + O(\lambda^2). \tag{5.16}$$

6 Extending the method

The second subsidiary goal of this paper is to show several extensions to this method and invite research into even more applications of Lie algebras into physics.

6.1 Simple one-dimensional corollaries

Now that we have given explicit formulae for computing perturbation eigenvalues for potentials of the form λx^n, we can extend by linearity (up to order one) and immediately recover eigenvalues for polynomial potentials. In fact, we can extend this further to convergent power series.

Example 14. Let us consider

$$H = a^\dagger a + \frac{1}{2} + \lambda e^x.$$

Of course this can be rewritten as

$$H = a^\dagger a + \frac{1}{2} + \lambda \left(\sum_k \frac{x^k}{k!} \right).$$

If we notice that only the even powered potentials contribute perturbations up to first order, then we will also compute perturbations for $H = H_0 + \lambda \cosh(x)$ as well.

Let us compute only the ground state energy. We have

$$E_0 = \frac{1}{2} + \lambda \left(\sum_k \frac{(2k)!}{2^{2k} k!(2k)!} \right) = \frac{1}{2} + \lambda \left(\sum_k \frac{4^{-k}}{k!} \right) = \frac{1}{2} + \lambda \exp(1/4).$$

Moreover, we can add any number of perturbation parameters and solve the system accordingly. In particular, we can essentially read off first-order perturbations for Hamiltonians of the form

$$H = H_0 + \sum_{j=1}^{n} \lambda_j x^{k_j}.$$

6.2 Simple N-dimensional corollaries

In extending this method, it is natural to ask whether one can tackle higher dimensional systems with a similar approach. In our case, we certainly can attack higher dimensional problems similarly, but the construction of the Lie algebra is different. For the simple N-dimensional corollaries, we will assume that our oscillator potential is not coupled (i.e. no terms of the form $\lambda x^j y^k$ appear). For the sake of simplicity, let us go through the construction of the Lie algebras for a two-dimensional oscillator.

Consider

$$H_{n,m} = a_x^\dagger a_x + \frac{1}{2} + \lambda_1 x^n + a_y^\dagger a_y + \frac{1}{2} + \lambda_2 y^m.$$

We will take four elements as given in our Lie algebra:

$$H_{0,0} = a_x^\dagger a_x + \frac{1}{2} + a_y^\dagger a_y + \frac{1}{2}, \quad H_{0,m} = H_{0,0} + \lambda_2 y^m,$$
$$H_{n,0} = H_{0,0} + \lambda_1 x^n, \quad H_{n,m} = H_{0,0} + \lambda_1 x^n + \lambda_2 y^m.$$

In this way, we will set up our Lie algebra as two independent oscillator Lie algebras and solve our problems from before. Consider for example

$$H_{1,4} = H_{0,0} + \lambda_1 x + \lambda_2 y^4.$$

Our Lie algebra $\mathcal{A}_{1,4}^{(1,1)}$ will have the following elements:

$$\begin{array}{lll} H_{0,0}, & H_{1,0}, & \lambda_1 \big(a_x^\dagger - a_x \big), \\ H_{0,4}, & H_{1,4}, & I, \\ \lambda_2 \big(a_y^{\dagger 4} - a_y^4 \big), & \lambda_2 \big(a_y^{\dagger 3} a_y - a_y^\dagger a_y^3 \big), & \lambda_2 \big(a_y^{\dagger 2} - a_y^2 \big), \\ \lambda_2 \big(a_y^{\dagger 4} + a_y^4 \big), & \lambda_2 \big(a_y^{\dagger 3} a_y + a_y^\dagger a_y^3 \big), & \lambda_2 \big(a_y^{\dagger 2} + a_y^2 \big). \end{array}$$

Our unitary takes the form

$$U=\exp\left(\alpha\lambda_1\left(a_x^\dagger-a_x\right)+\beta_1\lambda_2\left(a_y^{\dagger 4}-a_y^4\right)+\beta_2\lambda_2\left(a_y^{\dagger 3}a_y-a_y^\dagger a_y^3\right)+\beta_3\lambda_2\left(a_y^{\dagger 2}-a_y^2\right)\right).$$

Now we use the Hadamard lemma again, but taking advantage of the relations

$$\left[a_j^\dagger,a_k\right]=\delta_{jk} \tag{6.1}$$

we can completely separate x variables from y variables and our calculation plays out exactly as before.

For the Hamiltonian $H_{1,4}$ our perturbed ground state is

$$E_0=\frac{1}{2}+O\left(\lambda_1^2\right)+\frac{1}{2}+\frac{3\lambda_2}{4}+O\left(\lambda_2^2\right).$$

Now we can use all the simple one-dimensional corollaries in turn as well.

6.3 Higher-order perturbations

Since perturbation theory is meant to compute more than first-order terms, we seek to use this Lie algebraic method to compute higher-order terms. Certainly, one can see that using the transformations U we have set up thus far will produce higher order terms. One can see this if we set

$$U=\exp(\lambda L).$$

Our transformation becomes

$$U^\dagger H_0U=H_0+\lambda\left[H_0,L\right]-\frac{\lambda^2}{2}\left[L,\left[H_0,L\right]\right]\cdots. \tag{6.2}$$

This approach, however, changes our Hamiltonian fundamentally. In fact, we end up not solving any problems, but instead creating more. A quick trial calculation with any Hamiltonian carrying term x^3 or higher will reveal that we cannot cancel certain terms arising from $[L,[L,H_0]]$. To remove this difficulty, we must expand our Lie algebra to include terms carrying λ^k for whichever k we should choose. It is therefore convenient to write our unitary transformation as

$$U=\exp\left(\sum_{j=1}^{k}\lambda^j L_{(j)}\right), \tag{6.3}$$

where $L_{(j)}$ are Lie algebra elements arising from jth order commutators.

Example 15. Let us return briefly to the quartic oscillator and calculate its second-order perturbation. Since it is well studied, we may verify our results easily.

Computing commutators and commutators of commutators, one will arrive at the following Lie algebra up to order 2.

$$\begin{array}{lll}
H_0, & H_4, & I, \\
\lambda\left(a^{\dagger 4}\pm a^4\right), & \lambda\left(a^{\dagger 3}a\pm a^\dagger a^3\right), & \lambda\left(a^{\dagger 2}\pm a^2\right), \\
\lambda^2\left(a^{\dagger 6}\pm a^6\right), & \lambda^2\left(a^{\dagger 4}a^2\pm a^{\dagger 2}a^4\right), & \\
\lambda^2\left(a^{\dagger 4}\pm a^4\right), & \lambda^2\left(a^{\dagger 3}a\pm a^\dagger a^3\right), & \lambda^2\left(a^{\dagger 2}\pm a^2\right).
\end{array}$$

Knowing the form of our necessary first-order transformation, we add four terms to the exponential by

$$\begin{aligned}
U=\exp\Bigg(&\lambda\left(\frac{1}{16}\left(a^{\dagger 4}-a^4\right)+\frac{1}{2}\left(a^{\dagger 3}a-a^\dagger a^3\right)+\frac{3}{4}\left(a^{\dagger 2}-a^2\right)\right)+\lambda^2\beta_1\left(a^{\dagger 6}-a^6\right) \\
&+\lambda^2\beta_2\left(a^{\dagger 4}a^2-a^{\dagger 2}a^4\right)+\lambda^2\beta_3\left(a^{\dagger 3}a-a^\dagger a^3\right)+\lambda^2\beta_4\left(a^{\dagger 2}-a^2\right)\Bigg), \qquad (6.4)\\
U=\exp&\left(\lambda L_{(1)}+\lambda^2 L_{(2)}\right).
\end{aligned}$$

For simplicity, let us compute only the ground state energy given by $U^\dagger H_0 U$. We have

$$\begin{aligned} U^\dagger H_0 U &= \exp\left(-\lambda L_{(1)} - \lambda^2 L_{(2)}\right) H_0 \exp\left(\lambda L_{(1)} + \lambda^2 L_{(2)}\right) \\ &= H_0 + \lambda\left[H_0, L_{(1)}\right] + \lambda^2\left[H_0, L_{(2)}\right] - \frac{\lambda^2}{2}\left[L_{(1)}, \left[H_0, L_{(1)}\right]\right] + O\left(\lambda^3\right). \end{aligned}$$

From here it is a matter of computing commutators and adjusting $\beta_1, \beta_2, \beta_3, \beta_4$ to cancel higher order terms not given as functions of number operators.

When we compute the ground state energy, we are concerned only with constant terms. Therefore, looking to our commutators we have the λ^2 term

$$\left[\frac{1}{16}\left(a^{\dagger 4} - a^4\right) + \frac{1}{2}\left(a^{\dagger 3}a - a^\dagger a^3\right) + \frac{3}{4}\left(a^{\dagger 2} - a^2\right), \frac{1}{4}\left(a^{\dagger 4} + a^4\right) + \left(a^{\dagger 3}a + a^\dagger a^3\right) + \frac{3}{2}\left(a^{\dagger 2} + a^2\right)\right].$$

Expanding this we are left with two terms giving constants:

$$\frac{1}{64}\left[a^{\dagger 4} - a^4, a^{\dagger 4} + a^4\right] \quad \text{and} \quad \frac{9}{8}\left[a^{\dagger 2} - a^2, a^{\dagger 2} + a^2\right].$$

Our constant terms turn out to be $\frac{-2(4!)}{64}$ and $\frac{-2(2!)9}{8}$ yielding $\frac{-21}{4}$.

Finally, our ground state energy up to second order will be given by

$$\left(U^\dagger H_0 U\right) U^\dagger |0\rangle = \left(H_4 - \frac{3\lambda}{4} - \frac{-21}{4}\frac{\lambda^2}{2}\right) U^\dagger |0\rangle, \tag{6.5}$$

yielding

$$E_0 = \frac{1}{2} + \frac{3\lambda}{4} - \frac{21\lambda^2}{8} + O\left(\lambda^3\right). \tag{6.6}$$

Indeed, this ground state energy agrees with the standard perturbation theory.

For the interested reader, the correct β parameter values are

$$\beta_1 = \frac{1}{48}, \quad \beta_2 = \frac{-9}{16}, \quad \beta_3 = \frac{-9}{4}, \quad \beta_4 = \frac{-63}{32},$$

and the second-order equation appears as

$$U^\dagger H_0 U = H_4 - \frac{3\lambda}{2} N(N+1) - \frac{3\lambda}{4} + 51\lambda^2 \binom{N}{3} + \frac{117\lambda^2}{2}\binom{N}{2} + 36\lambda^2 N + \frac{21\lambda^2}{8} + O\left(\lambda^3\right). \tag{6.7}$$

7 Discussion

One important problem among many arising from this paper and which we have yet neglected to mention is the representation theory of the Lie algebras. For example, if we are dealing with the cases λx, λx^2 in the one-dimensional case or any quadratic term in higher dimensional cases, we have a closed Lie algebra. This may not be terribly surprising as a closed Lie algebra offers an exact solution, and these particular potentials are simply shifted or coupled harmonic oscillators. However, the Lie algebras we have constructed all contain central elements. In the cases of $\mathcal{A}_1$ and $\mathcal{A}_2$ we have 4-dimensional closed Lie algebras with center. Representation theory tells us that these are isomorphic to $\mathfrak{gl}_2$. It remains to be seen exactly the relationship between these Lie algebras and the symmetries they describe. In this paper, we have only used them to calculate perturbed energy levels. It is entirely possible that there is a simpler approach to this problem from an entirely representation theoretic standpoint.

As it stands, we have given explicit constructions for Lie algebras up to any order and the method by which we may construct a unitary operator to make the transformation

$$H_0 \longmapsto H_n + \text{perturbations up to } O\left(\lambda^k\right).$$

By taking advantage of our symmetric construction of these Lie algebras, the Hadamard lemma, and several formulae concerning abstract Weyl algebras, we have managed to give eigenvalues in agreement with standard methods.

Another issue which we have neglected to resolve is how to deal with coupled oscillators in general. In the appendix, we briefly mention the way to deal with potentials of the form λxy. The Lie algebra computations for coupling terms of the form $\lambda x^n y^m$ are more taxing and trickier. This method, however, should be able to deal with situation, but some coordinate change may be required first.

It is the hope of the author that anharmonic oscillators are simply a useful class of examples for the propitiation of this method. Furthermore, it is hoped that this method will help to give rise to additional representation theoretic methods in physics.

Appendix: dealing with harmonic oscillators

Two important cases we have not touched upon are those of actual harmonic oscillators in one and multiple dimensions. Consider, for example, the two Hamiltonians

$$H_2 = a^\dagger a + \frac{1}{2} + \lambda\left(\frac{a^\dagger + a}{\sqrt{2}}\right)^2, \quad H_c = a_x^\dagger a_x + a_y^\dagger a_y + 1 + \frac{\lambda}{2}\left(a_x^\dagger + a_x\right)\left(a_y^\dagger + a_y\right). \tag{7.1}$$

These correspond to the shifted frequency oscillator in one dimension with new frequency $\sqrt{1+2\lambda}$ and a coupled oscillator in two dimensions with quadratic coupling term. These cases have been well studied and so we have neglected them thus far. However, the techniques to compute the perturbations are special because these Hamiltonians along with H_0 and $H_{0,0}$ produce closed Lie algebras. By our theorem earlier, we know that we can solve these exactly and not concern ourselves with kth order perturbations.

The main technique we employ is to transform our ladder operators via the so-called Bogoliubov transforms. In one dimension, we have

$$b^\dagger = U^\dagger a^\dagger U = \sigma a^\dagger + \tau a, \quad b = U^\dagger a U = \sigma a + \tau a^\dagger. \tag{7.2}$$

In this way, we produce the new Hamiltonian

$$\sqrt{1+2\lambda}\left(b^\dagger b + \frac{1}{2}\right) = a^\dagger a + \frac{1}{2} + \frac{\lambda}{2}\left(a^\dagger + a\right)^2.$$

This algebra to move from σ, τ to this clean form of the new Hamiltonian is tedious to be sure. The interested reader should confer with [2] or email the author for a small set of notes.

A similar technique can be used for the quadratic coupling, but the transformation must take into account much more coupling. Our transformation should look something like

$$\begin{pmatrix} b_x^\dagger \\ b_x \\ b_y^\dagger \\ b_y \end{pmatrix} = \begin{pmatrix} \alpha & \beta & \gamma & \delta \\ \beta & \alpha & \delta & \gamma \\ \sigma & \tau & \mu & \nu \\ \tau & \sigma & \nu & \mu \end{pmatrix} \begin{pmatrix} a_x^\dagger \\ a_x \\ a_y^\dagger \\ a_y \end{pmatrix}. \tag{7.3}$$

This is simply a coordinate change which decouples the coordinate variables. The matrix, however, will take a very special form so that $[b_i, b_j^\dagger] = \delta_{ij}$ as did the initial coordinates.

Remark 16. Notice here that we can couple our ladder operators in many more ways in agreement with [1]. For example, we can tackle problems such as dynamic coupling

$$H = x^2 - \partial_x^2 + y^2 - \partial_y^2 + \lambda \partial_x \partial_y,$$

or oscillators in a magnetic field

$$H = x^2 - \partial_x^2 + y^2 - \partial_y^2 + \lambda\left(y\partial_x - x\partial_y\right).$$

So long as our coupling term contains terms of order two or less in each of the ladder operators, we can tackle these problems with a simple coordinate change.

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