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Frequency operator for anharmonic oscillators

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Abstract
We develop a simple approach based on time-independent perturbation theory that leads to a frequency operator for quantum mechanical models. This method is suitable for the calculation of time-dependent physical properties free from secular terms. In particular we obtain the first-order perturbation correction to the frequency operator for a class of anharmonic oscillators.

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1. Introduction

In a recent paper Pathak [1] applied first-order perturbation theory to the Heisenberg equations of motion for quantum mechanical anharmonic oscillators in order to generalize previous results derived by means of multiple-scale analysis [2, 3]. Such an approximation leads to a sort of frequency operator that plays the role of the frequency of periodic motion in classical mechanics, and produces results free from secular terms. Because of the renewed interest in this kind of approximation, here we develop a simpler method for the straightforward derivation of analytic expressions for the frequency operator for general quantum mechanical anharmonic oscillators.

2. Method

Given a quantum mechanical system with Hamiltonian operator $\hat{H}$ we try to solve the equation

$$[\hat{H}, \hat{b}] = -\hat{\Omega}\hat{b} \tag{1}$$

where $[\hat{A}, \hat{B}] = \hat{A}\hat{B} - \hat{B}\hat{A}$ is the commutator between linear operators $\hat{A}$ and $\hat{B}$, and $\hat{\Omega} = \hat{\Omega}^\dagger$ is a constant of the motion:

$$[\hat{H}, \hat{\Omega}] = 0. \tag{2}$$

Under such conditions, the time evolution of the operator $\hat{b}$ is

$$\hat{b}(t) = \exp\left(-\frac{\mathrm{i}t}{\hbar}\hat{\Omega}\right)\hat{b} \tag{3}$$

where $\hat{b}(0) = \hat{b}$ [4]. Since equation (1) does not determine the operator $\hat{b}$ completely [4], we should add a *normalization condition*, such as $[\hat{b}, \hat{b}^\dagger] = \hat{1}$ or $\hat{H} = \hat{b}^\dagger\hat{b} + e\hat{1}$, where e is a real number. From now on we omit the identity operator $\hat{1}$ and simply write 1 instead, when necessary.

Bacus *et al* [5] proposed a solution to an equation similar to (1) in the form of an operator series, with a convenient operator ordering. They were able to obtain remarkably accurate eigenvalues for an anharmonic oscillator from a Riccati equation derived from that approach in the coordinate representation. Here we try a different approach based on perturbation theory. To this end, we write

$$\hat{H} = \hat{H}_0 + \lambda\hat{H}' \tag{4}$$

and look for solutions in the form of power series:

$$\hat{\Omega} = \sum_{j=0}^{\infty} \hat{\Omega}_j\lambda^j \tag{5a}$$

$$\hat{b} = \sum_{j=0}^{\infty} \hat{b}_j\lambda^j. \tag{5b}$$

One easily verifies that the coefficients $\hat{\Omega}_j$ and $\hat{b}_j$ satisfy the perturbation equations

$$[\hat{H}_0, \hat{\Omega}_j] + [\hat{H}', \hat{\Omega}_{j-1}] = 0 \tag{6a}$$

$$[\hat{H}_0, \hat{b}_j] + \hat{\Omega}_0\hat{b}_j = [\hat{b}_{j-1}, \hat{H}'] - \sum_{i=1}^{j} \hat{\Omega}_i\hat{b}_{j-i} \tag{6b}$$

as follows from equations (2) and (1), respectively. We assume that we can solve the equations of order zero $[\hat{H}_0, \hat{b}_0] = -\hat{\Omega}_0\hat{b}_0$ and $[\hat{H}_0, \hat{\Omega}_0] = 0$ exactly. Equation (6*a*) determines $\hat{\Omega}_j$ except for terms $\hat{U}_j$ that commute with $\hat{H}_0$. All the terms in the right-hand side of equation (6*b*), except the unknown part $\hat{U}_j$ of $\hat{\Omega}_j$, were obtained in previous steps. In order to solve equation (6*b*), its right-hand side should be free from 'secular' terms $\hat{Z}_j$ that satisfy the unperturbed equation

$$[\hat{H}_0, \hat{Z}_j] + \hat{\Omega}_0\hat{Z}_j = 0 \tag{7}$$

and would give rise to singularities. Since $\hat{U}_j\hat{b}_0$ satisfies the latter equation, we set $\hat{U}_j$ in order to remove the unwanted terms. We can then solve equation (6*b*) for $\hat{b}_j$ which is therefore completely determined up to terms that satisfy equation (7). We obtain the latter by means of an appropriate normalization condition as mentioned earlier. It will not be necessary for our present goal, which is the calculation of $\hat{\Omega}_1$. At first order in λ we have

$$[\hat{H}_0, \hat{\Omega}_1] + [\hat{H}', \hat{\Omega}_0] = 0 \tag{8a}$$

$$[\hat{H}_0, \hat{b}_1] + \hat{\Omega}_0\hat{b}_1 = [\hat{b}_0, \hat{H}'] - \hat{\Omega}_1\hat{b}_0. \tag{8b}$$

Solving these perturbation equations for anharmonic oscillators offers no difficulty. For simplicity, in what follows we choose dimensionless one-dimensional operators of the form

$$\hat{H} = \frac{1}{2}\hat{p}^2 + \frac{1}{2}\hat{x}^2 + \frac{\lambda}{m}\hat{x}^m \qquad m = 4, 6, \ldots \tag{9}$$

where $[\hat{x}, \hat{p}] = \mathrm{i}$. It is convenient to express the perturbation equations in terms of the creation $\hat{a}^\dagger$ and annihilation $\hat{a}$ boson operators that satisfy the commutation relation $[\hat{a}, \hat{a}^\dagger] = 1$. We choose

$$\hat{H}_0 = \hat{a}^\dagger\hat{a} + \tfrac{1}{2} \tag{10}$$

and

$$\hat{H}' = \frac{1}{m}\hat{x}^m = \frac{1}{2^{m/2}m}(\hat{a} + \hat{a}^\dagger)^m \tag{11}$$

so that $\hat{b}_0 = \hat{a}$ and $\hat{\Omega}_0 = 1$. Equation (8a) reduces to $[\hat{H}_0, \hat{\Omega}_1] = 0$, which tells us that $\hat{\Omega}_1$ is a function of $\hat{H}_0$. In order to solve equation (8b) we choose $\hat{\Omega}_1$ in such a way that the right-hand side of that equation is free from terms $\hat{Z}_1$ that satisfy equation (7) with $j = 1$.

When working with the boson algebra it is customary to choose normal order in which the creation operator appears to the left of the annihilation operator everywhere. To this end Pathak developed a lengthy procedure in order to write $\hat{x}^m$ in normal order [1]. Here, we make use of a much simpler algorithm that consists of expanding a power of $\hat{x}$ in the form of a recurrence relation [6]:

$$\hat{x}^k = \frac{1}{\sqrt{2}}(\hat{a}^\dagger\hat{x}^{k-1} + \hat{x}^{k-1}\hat{a}) + \frac{k-1}{2}\hat{x}^{k-2} \qquad k = 2, 3, \ldots. \tag{12}$$

Notice that $\hat{x}^0 = 1$ and $\hat{x}^1 = \hat{x}$ are in normal order, and that if both $\hat{x}^{k-1}$ and $\hat{x}^{k-2}$ are in normal order, then $\hat{x}^k$ is in normal order too. By means of this recurrence relation we manipulate the boson operators as if they were mere numbers because the normal order is always granted. For example, if $\hat{H}'$ is in normal order, then we can formally write $[\hat{a}, \hat{H}'] = \frac{\partial \hat{H}'}{\partial \hat{a}^\dagger}$, where the derivative is carried out in the usual way. Proceeding as indicated it is clear that we can safely ignore that the boson operators do not commute when solving equation (8b). This fact greatly facilitates the calculation of analytic expressions of $\hat{\Omega}_1$ for any desired value of m. Because the procedure becomes tedious even for moderately great m, it is advisable to make use of available software for symbolic computation, like Maple$^{\mathrm{TM}}$.

The operator $\hat{\Omega}_1\hat{a}$ is a linear combination of terms of the form $(\hat{a}^\dagger)^j\hat{a}^{j+1}$ because $\hat{\Omega}_1$ is a polynomial function of $\hat{a}^\dagger\hat{a}$. Notice that $P(\hat{a}^\dagger, \hat{a}) = [\hat{a}, \hat{H}']$ is a polynomial function of the creation and annihilation operators with monomials $(\hat{a}^\dagger)^j\hat{a}^k$, and that

$$\int_0^{2\pi} \mathrm{e}^{\mathrm{i}t}(\mathrm{e}^{\mathrm{i}t}\hat{a}^\dagger)^j(\mathrm{e}^{-\mathrm{i}t}\hat{a})^k\,\mathrm{d}t = 2\pi\delta_{k\ j+1}(\hat{a}^\dagger)^j\hat{a}^k. \tag{13}$$

Therefore, we easily obtain $\hat{\Omega}_1$ by means of the equation

$$\hat{\Omega}_1\hat{a} = \int_0^{2\pi} \mathrm{e}^{\mathrm{i}t}P(\mathrm{e}^{\mathrm{i}t}\hat{a}^\dagger, \mathrm{e}^{-\mathrm{i}t}\hat{a})\,\mathrm{d}t \tag{14}$$

where once again the normal order allows us to treat boson operators as mere numbers. Using this simple recipe we easily obtain $\hat{\Omega}_1$ for any anharmonic oscillator as a polynomial with monomials $(\hat{a}^\dagger)^j\hat{a}^j$. In order to express such results in terms of $\hat{H}_0$ we have to rewrite that polynomial in terms of monomials $(\hat{a}^\dagger\hat{a})^j$. To this end, we expand both sides of the well known disentangling formula [6]

$$\exp(\theta\hat{a}^\dagger\hat{a}) = \sum_{j=0}^{\infty}\frac{(\mathrm{e}^\theta - 1)^j}{j!}(\hat{a}^\dagger)^j\hat{a}^j \tag{15}$$

in a Taylor series about $\theta = 0$, and compare like coefficients.

Table 1 shows $\hat{\Omega}_1(\hat{H}_0)$ for the anharmonic oscillators (9) with $m = 2, 4, \ldots, 14$. We have purposely included the exactly solvable harmonic perturbation $m = 2$ in order to test our algorithm. In this case one easily proves that the frequency operator is a real number $\hat{\Omega} = \Omega = \sqrt{1+\lambda}$ for all $\lambda > -1$ (remember that we omit the identity operator). The coefficient of the linear term of the Taylor expansion $\Omega = 1 + \frac{\lambda}{2} - \frac{\lambda^2}{8} + \cdots$ agrees with the value of $\hat{\Omega}_1$ for $m = 2$ in table 1, showing that our approach gives the correct answer for this

Table 1. Perturbation correction $\hat{\Omega}_1$ to the frequency operator for the anharmonic oscillators $\hat{H} = \frac{1}{2}\hat{p}^2 + \frac{1}{2}\hat{x}^2 + \frac{\lambda}{m}\hat{x}^m$.

m	$\hat{\Omega}_1$
2	$\frac{1}{2}$
4	$\frac{3}{4}\hat{H}_0 + \frac{3}{8}$
6	$\frac{5}{4}\hat{H}_0^2 + \frac{5}{4}\hat{H}_0 + \frac{15}{16}$
8	$\frac{35}{16}\hat{H}_0^3 + \frac{105}{32}\hat{H}_0^2 + \frac{385}{64}\hat{H}_0 + \frac{315}{128}$
10	$\frac{63}{16}\hat{H}_0^4 + \frac{63}{8}\hat{H}_0^3 + \frac{819}{32}\hat{H}_0^2 + \frac{693}{32}\hat{H}_0 + \frac{2835}{256}$
12	$\frac{231}{32}\hat{H}_0^5 + \frac{1155}{64}\hat{H}_0^4 + \frac{5775}{64}\hat{H}_0^3 + \frac{15\,015}{128}\hat{H}_0^2 + \frac{71\,379}{512}\hat{H}_0 + \frac{51\,975}{1024}$
14	$\frac{429}{32}\hat{H}_0^6 + \frac{1287}{32}\hat{H}_0^5 + \frac{36\,465}{128}\hat{H}_0^4 + \frac{32\,175}{64}\hat{H}_0^3 + \frac{522\,951}{512}\hat{H}_0^2 + \frac{397\,683}{512}\hat{H}_0 + \frac{675\,675}{2048}$

model. In order to check the expressions of $\hat{\Omega}_1$ for anharmonic oscillators that we cannot solve exactly, we simply take into account that those operators satisfy

$$E_{n+1,1} - E_{n,1} = \langle n|\hat{\Omega}_1|n\rangle \tag{16}$$

where $E_{n,1}$ is the perturbation correction of first order to the eigenvalue with quantum number n, and $|n\rangle$ is the corresponding eigenvector of the number operator $\hat{a}^\dagger\hat{a}$. For example, for the quartic oscillator $m = 4$ we have [7]

$$E_{n,1} = \frac{3}{8}n^2 + \frac{3}{8}n + \frac{3}{16} \tag{17}$$

and

$$E_{n+1,1} - E_{n,1} = \langle n|\hat{\Omega}_1|n\rangle = \frac{3}{4}(n+1). \tag{18}$$

Our expressions for $\hat{\Omega}_1$ given in table 1 do not agree with Pathak's [1] because the frequency operator derived here by a pure operator method and perturbation theory is not exactly the one that we should insert into the multiple-scale equations [2, 3]. Notice, for example, that the expressions for the latter approach exhibit cosines in the denominators with the perturbation parameter in their arguments [2,3]. Obviously, perturbation theory expands such trigonometric functions in Taylor series and, consequently, they do not appear in the resulting perturbation corrections that are independent of that parameter.

At first order we should write

$$\hat{b}(t) \simeq \exp[-\mathrm{i}t(1 + \lambda\hat{\Omega}_1)]\hat{a} + \lambda\exp(-\mathrm{i}t)\hat{b}_1. \tag{19}$$

Since $\hat{b}_1$ is independent of time, this equation is free from secular terms. If for simplicity we omit the second term from the right-hand side of this equation, and take into account that under such a condition $\hat{b} \simeq \hat{a}$, then we obtain

$$\hat{x}(t) \simeq \frac{1}{2}[\exp(-\mathrm{i}t\hat{\Omega})\hat{x} + \hat{x}\exp(\mathrm{i}t\hat{\Omega})] + \frac{\mathrm{i}}{2}[\exp(-\mathrm{i}t\hat{\Omega})\hat{p} - \hat{p}\exp(\mathrm{i}t\hat{\Omega})] \tag{20}$$

where $\hat{\Omega} \simeq 1 + \lambda\hat{\Omega}_1$. This equation is similar to those derived earlier [1–3], except for the cosine denominators mentioned above.

3. Conclusions

We have presented a straightforward approach for the calculation of the frequency operator for quantum mechanical anharmonic oscillators. The main advantage of our perturbation method is that at first order it circumvents the noncommuting algebra of the boson operators, which we can thus treat as mere numbers. This fact greatly facilitates solving the perturbation equations, specially for large anharmonic exponents m. However, at second order the situation is completely different, and we have to take into account the order of the operators explicitly. Moreover, the perturbation corrections of order greater than unity to the frequency operator do not commute with $\hat{H}_0$, and are therefore more difficult to include in the calculation of physical properties, particularly because they appear in the exponential term $\exp(-\frac{it}{\hbar}\hat{\Omega})$, which we should not expand in a Taylor series if we do not want to generate secular terms [8]. This fact is probably the reason why most approaches developed to avoid secular terms in quantum mechanical time-dependent perturbation theory do not go beyond the first order [1–3]. It is worth mentioning, however, that the simple and straightforward ordering algorithm given by equation (12) is still useful at these higher perturbation orders.

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