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Frequency operator for anharmonic oscillators by perturbation theory

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Abstract
We obtain approximate analytical expressions for the frequency operator for anharmonic oscillators by means of perturbation theory and a unitary transformation.

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1. Introduction

Straightforward application of perturbation theory to nonlinear equations of motion in classical mechanics gives rise to secular terms that increase unboundedly with time even for periodic motion [1–3]. The Lindstedt–Poincaré technique, the method of renormalization and the method of multiple scales are some of the approaches that enable one to correct such unphysical behaviour of the approximate solutions [1–3]. The actual frequency of the motion, which appears explicitly as a natural consequence of the application of those procedures, plays an important role in the perturbation calculation.

Unphysical secular terms also appear in the application of time-dependent perturbation theory to quantum-mechanical systems. In order to remove them, several authors have adapted the methods of classical mechanics mentioned above and applied them to anharmonic oscillators as simple illustrative examples. The methods of Lindstedt–Poincaré and Bogoliubov and Krylov [4, 5], multiple-scale analysis [6–8], the renormalization-group method [9], a near-identity transformation [10], Taylor series approach [11, 12], normal ordering technique [13] and a time-independent eigenoperator method [14, 15] have proved suitable for this purpose. In these approaches the counterpart of the classical frequency is played by a q-number renormalized frequency or frequency operator.

Bender and Bettencourt's recent papers [6, 7] have motivated the interest in the equations of motion for the Heisenberg operators for the one-dimensional quartic anharmonic oscillator

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[8–15]. These authors generalized the method of multiple scales and obtained a frequency operator in terms of the unperturbed Hamiltonian that they interpreted as an operator form of mass renormalization that provides the first-order shift of energy differences [6, 7]. It does not appear to be well known that much earlier Aks [4] and Aks and Carhart [5] had also derived a q-number renormalized frequency for the Heisenberg position operator that they also interpreted as a kind of mass renormalization. Other authors showed marked interest in the quartic anharmonic oscillator; for example, Mandal [11] proposed a Taylor series method, Egusquiza and Valle Basagoiti [9] resorted to a renormalization-group technique, and Kahn and Zarmi [10] developed a near-identity transformation. Later, Pathak [13] generalized first-order results from quartic to higher anharmonicity, and Fernández [14, 15] obtained expressions of first order for general anharmonic oscillators and of second order for the quartic case.

Unlike the frequency in classical mechanics, the frequency operator for quantum-mechanical models does not appear to be uniquely defined, as shown by the fact that different methods may produce seemingly different frequency operators [4–7, 9–15]. The reason is that the form of the frequency operator in the resulting expressions depends on its relative position with respect to other operators that do not commute with it.

By means of a most interesting nonperturbative approach, Speliotopoulos [16] derived an expression for the frequency operator in terms of the Hamiltonian of a quartic anharmonic oscillator valid through second order of perturbation theory. The purpose of this paper is to generalize Speliotopoulos's result to other anharmonic oscillators and to higher perturbation orders. In section 2 we outline the frequency-operator method in much the same way Speliotopoulos did [16]. In section 3 we derive approximate expressions for the frequency operator for anharmonic oscillators by means of perturbation theory and a unitary transformation.

2. The frequency-operator method

The frequency-operator method is based on a straightforward generalization of the harmonic-oscillator algebra for the creation and annihilation boson operators [16]. Given the Hamiltonian operator $\hat{H}$, we look for an operator $\hat{b}$ that satisfies the following equations [14–16]:

$$\begin{aligned} &[\hat{H},\hat{b}] = -\hat{\Omega}\hat{b} \\ &[\hat{H},\hat{\Omega}] = 0 \qquad \hat{\Omega}^\dagger = \hat{\Omega} \end{aligned} \tag{1}$$

where $\hat{\Omega}$ is the frequency operator. In order to avoid unnecessary complications, we assume that the complete set of commuting observables is simply given by the Hamiltonian operator, so that any operator that commutes with $\hat{H}$ is a function of it. In the particular case of the frequency operator, we have $\hat{\Omega} = \Omega(\hat{H})$.

The adjoint of $\hat{b}$ satisfies

$$[\hat{H},\hat{b}^\dagger] = \hat{b}^\dagger\hat{\Omega}. \tag{2}$$

Note that equations (1) and (2) do not determine the operators $\hat{b}$ and $\hat{b}^\dagger$ completely. In fact, $\hat{W}\hat{b}$ satisfies equation (1) for any operator $\hat{W}$ that commutes with $\hat{H}$.

If we rewrite the operator equation $e^{\alpha\hat{H}}\hat{b}\,e^{-\alpha\hat{H}} = e^{-\alpha\hat{\Omega}}\hat{b}$ as $e^{\alpha(\hat{H}+\hat{\Omega})}\hat{b} = \hat{b}\,e^{\alpha\hat{H}}$, expand both sides in powers of α and compare the coefficients of the same power of this parameter, we conclude that $(\hat{H}+\hat{\Omega})^k\hat{b} = \hat{b}\hat{H}^k$. Therefore, if we can expand the function $F(\hat{H})$ in a formal power series of $\hat{H}$, we obtain

$$\hat{b}F(\hat{H}) = F(\hat{H}+\hat{\Omega})\hat{b} \quad \Rightarrow \quad [\hat{b}, F(\hat{H})] = [F(\hat{H}+\hat{\Omega}) - F(\hat{H})]b. \tag{3}$$

Analogously, we have

$$F(\hat{H})\hat{b}^\dagger = \hat{b}^\dagger F(\hat{H}+\hat{\Omega}) \quad \Rightarrow \quad [F(\hat{H}), \hat{b}^\dagger] = \hat{b}^\dagger[F(\hat{H}+\hat{\Omega}) - F(\hat{H})]. \tag{4}$$

If we define the function $F(k, \hat{H})$ as

$$\hat{b}^k F(\hat{H}) = F(k, \hat{H})\hat{b}^k \qquad F(0, \hat{H}) = F(\hat{H}) \tag{5}$$

it follows from $\hat{b}^k F(\hat{H}) = \hat{b}F(k-1, \hat{H})\hat{b}^{k-1} = F(k-1, \hat{H}+\hat{\Omega})\hat{b}^k$ that

$$F(k, \hat{H}) = F(k-1, \hat{H}+\hat{\Omega}) \qquad k = 1, 2, \ldots. \tag{6}$$

From this recurrence relation, we easily obtain $F(k, \hat{H})$ for any value of k.

It is not difficult to prove that $\hat{b}^\dagger\hat{b}$ is a constant of motion:

$$[\hat{H}, \hat{b}^\dagger\hat{b}] = [\hat{H}, \hat{b}^\dagger]\hat{b} + \hat{b}^\dagger[\hat{H}, \hat{b}] = \hat{b}^\dagger\hat{\Omega}\hat{b} - \hat{b}^\dagger\hat{\Omega}\hat{b} = 0. \tag{7}$$

On the other hand,

$$[\hat{H}, \hat{b}\hat{b}^\dagger] = [\hat{b}\hat{b}^\dagger, \hat{\Omega}] \quad \Rightarrow \quad [\hat{H}+\hat{\Omega}, \hat{b}\hat{b}^\dagger] = 0. \tag{8}$$

Consider a complete set of eigenfunctions common to both operators $\hat{H}$ and $\hat{\Omega}$:

$$\hat{H}\Psi_n = E_n\Psi_n \qquad \hat{\Omega}\Psi_n = \Omega_n\Psi_n. \tag{9}$$

It follows from the hypervirial theorem

$$\langle\Psi_m|[\hat{H}, \hat{b}]|\Psi_n\rangle = (E_m - E_n)\langle\Psi_m|\hat{b}|\Psi_n\rangle \tag{10}$$

and equations (1) and (9) that

$$(E_m - E_n + \Omega_m)\langle\Psi_m|\hat{b}|\Psi_n\rangle = 0. \tag{11}$$

Since the operator $\hat{b}$ is nonzero, there must be a pair of states Ψ_m and Ψ_n such that $b_{mn} = \langle\Psi_m|\hat{b}|\Psi_n\rangle \neq 0$. We then realize that $\hat{\Omega}$ plays the role of a frequency operator because its eigenvalues are energy differences:

$$\Omega_m = \Omega(E_m) = E_n - E_m. \tag{12}$$

Speliotopoulos discussed other interesting properties of the frequency operator [16]. Here we mention that the time evolution of the operator $\hat{b}$ is simply given by ($\hbar = 1$ for dimensionless equations)

$$\hat{b}(t) = \mathrm{e}^{\mathrm{i}t\hat{H}}\hat{b}\,\mathrm{e}^{-\mathrm{i}t\hat{H}} = \mathrm{e}^{-\mathrm{i}t\hat{\Omega}}\hat{b} \tag{13}$$

and its matrix elements are periodic functions of time,

$$\langle\Psi_m|\hat{b}(t)|\Psi_n\rangle = \mathrm{e}^{-\mathrm{i}t\hat{\Omega}_m}\langle\Psi_m|\hat{b}|\Psi_n\rangle = \mathrm{e}^{\mathrm{i}t(E_m-E_n)}\langle\Psi_n|\hat{b}|\Psi_m\rangle. \tag{14}$$

For any sufficiently well-behaved operator function $\hat{O} = O(\hat{b}, \hat{b}^\dagger)$, we have

$$\mathrm{e}^{\mathrm{i}t\hat{H}}\hat{O}\,\mathrm{e}^{-\mathrm{i}t\hat{H}} = \hat{O}(\mathrm{e}^{-\mathrm{i}t\hat{\Omega}}\hat{b}, \hat{b}^\dagger\,\mathrm{e}^{\mathrm{i}t\hat{\Omega}}). \tag{15}$$

3. Approximate solutions by means of perturbation theory

It is not possible to solve equations (1) exactly, except for some trivial models. However, one can obtain approximate solutions by means of perturbation theory if it is possible to write $\hat{H} = \hat{H}_0 + \lambda\hat{H}'$ in such a way that one can exactly solve the relevant equations for $\hat{H}_0$. One easily proves that the coefficients of the expansions

$$\hat{\Omega} = \sum_{j=0}^{\infty}\hat{\Omega}_j\lambda^j \qquad \hat{b} = \sum_{j=0}^{\infty}\hat{b}_j\lambda^j \tag{16}$$

satisfy the operator equations [14, 15]

$$[\hat{H}_0, \hat{\Omega}_j] = [\hat{\Omega}_{j-1}, \hat{H}'] \qquad [\hat{H}_0, \hat{b}_j] + \hat{\Omega}_0\hat{b}_j = [\hat{b}_{j-1}, \hat{H}'] - \sum_{k=1}^{j} \hat{\Omega}_k\hat{b}_{j-k}. \tag{17}$$

In the particular case of anharmonic oscillators $\hat{H} = (\hat{p}^2 + \hat{x}^2)/2 + \lambda\hat{x}^{2m}/(2m)$, $\hat{\Omega}_0 = 1$ and $\hat{\Omega}_1$ commutes with the harmonic part $\hat{H}_0$. Fernández [14] has recently derived $\hat{\Omega}_1(\hat{H}_0)$ for several values of the anharmonicity exponent m and $\hat{\Omega}_1(\hat{H}_0)$ and $\hat{\Omega}_2(\hat{a}, \hat{a}^\dagger)$ for the quartic case $\hat{H} = \hat{a}^\dagger\hat{a} + 1/2 + \lambda(\hat{a}^\dagger + \hat{a})^4/16$ [14, 15]. By means of the method developed in this section and a semiclassical approach, Speliotopoulos obtained [16]

$$\begin{aligned} \hat{\Omega}(\hat{H}) &= 1 + 3\epsilon\left(\hat{H} + \tfrac{1}{2}\right) - \epsilon^2\left[\tfrac{69}{64}\left(\hat{H} + \tfrac{1}{2}\right)^2 - \tfrac{9}{2}\left(\hat{H} + \tfrac{1}{2}\right) + \tfrac{15}{2}\right] + \cdots \\ \hat{H} &= \hat{a}^\dagger\hat{a} + \frac{1}{2} + \frac{\epsilon}{4}(\hat{a}^\dagger + \hat{a})^4. \end{aligned} \tag{18}$$

which after expanding through order ϵ^2, and substituting $\epsilon = \lambda/4$, leads to the perturbation expansion derived by Fernández [15].

In what follows we propose a straightforward systematic derivation of the frequency operator $\hat{\Omega} = \Omega(\hat{H})$ by means of perturbation theory. The method is particularly simple because it avoids the operator equations (17) used in earlier approaches [14, 15]. Rayleigh–Schrödinger perturbation theory gives us the coefficients of the expansions [3]

$$E_n = \sum_{j=0}^{\infty} E_{n,j}\lambda^j \qquad \Psi_n = \sum_{j=0}^{\infty} \Psi_{n,j}\lambda^j \tag{19}$$

where $\Psi_{n,0} = \Phi_n$ and $E_{n,0} = \epsilon_n$ are the eigenvectors and eigenvalues of $\hat{H}_0$:

$$\hat{H}_0\Phi_n = \epsilon_n\Phi_n. \tag{20}$$

Following a recent application of multiple-scale techniques to anharmonic oscillators, we consider a unitary operator $\hat{T}$ that maps one set of eigenvectors onto the other [8]:

$$\Phi_n = \hat{T}\Psi_n \qquad \hat{T}^\dagger = \hat{T}^{-1}. \tag{21}$$

It follows from equations (9) and (21) that

$$\hat{\mathcal{H}}\Phi_n = E_n\Phi_n \qquad \hat{\mathcal{H}} = \hat{T}\hat{H}\hat{T}^\dagger. \tag{22}$$

Since $\hat{H}_0$ forms by itself a complete set of commuting observables for the unperturbed system, then $\hat{\mathcal{H}} = \mathcal{H}(\hat{H}_0)$, and $E_n = \mathcal{H}(\epsilon_n)$.

As a particular case we consider a one-dimensional anharmonic oscillator with Hamiltonian operator $\hat{H} = H(\hat{a}, \hat{a}^\dagger)$, where $H(x, y)$ is an analytical function of its arguments, and $\hat{a}$ and $\hat{a}^\dagger$ are the annihilation and creation boson operators, respectively, that satisfy $[\hat{a}, \hat{a}^\dagger] = 1$. An appropriate reference model for this problem is the harmonic oscillator

$$\hat{H}_0 = \hat{n} + \tfrac{1}{2} \tag{23}$$

where $\hat{n} = \hat{a}^\dagger\hat{a}$ is the occupation number operator. It follows from equation (22) that

$$\hat{\mathcal{H}} = \mathcal{H}(\hat{H}_0) = f(\hat{n}) \tag{24}$$

where $f(n) = E_n$. Taking into account that equation (3) becomes

$$[f(\hat{n}), \hat{a}] = -\hat{\omega}\hat{a} \qquad \hat{\omega} = \omega(\hat{n}) = f(\hat{n} + 1) - f(\hat{n}) \tag{25}$$

one easily proves that

$$[\hat{H}, \hat{T}^\dagger\hat{a}\hat{T}] = -\hat{T}^\dagger\hat{\omega}\hat{T}\hat{T}^\dagger\hat{a}\hat{T}. \tag{26}$$

Therefore, if we define

$$\hat{b} = b(\hat{a}, \hat{a}^\dagger) = \hat{T}^\dagger \hat{a} \hat{T} \qquad \hat{\Omega} = \hat{T}^\dagger \hat{\omega} \hat{T} \tag{27}$$

equation (26) becomes a particular case of equation (1). Note that the frequency operator $\hat{\Omega}$ given by equation (27) is already a constant of motion:

$$[\hat{H}, \hat{\Omega}] = \hat{T}^\dagger [f(\hat{n}), \omega(\hat{n})] \hat{T} = 0. \tag{28}$$

Under such conditions the first terms of the operator series (16) are $\hat{\Omega}_0 = 1$ and $\hat{b}_0 = \hat{a}$. One easily solves the perturbation equations for the coefficients $\hat{b}_j$ and $\hat{\Omega}_j$ with appropriate normalization conditions for the operators $\hat{b}$ and $\hat{b}^\dagger$ (which in this case should be $[\hat{b}, \hat{b}^\dagger] = 1$) [15]. The method is straightforward though tedious and applies to both the classical and quantum cases [15]. The relevant fact is that no secular terms appear when we substitute the perturbation series (16) into the time-evolution expressions (15).

The unitary transformation method just outlined provides a connection between a multiple-scale analysis and the frequency-operator method [21]. In what follows we derive $\hat{\Omega} = \Omega(\hat{H})$ by means of perturbation theory and generalize previous results for the quartic harmonic oscillator [16]. First of all note that

$$\hat{b}\Psi_n = \sqrt{n}\Psi_{n-1} \qquad \hat{b}^\dagger \Psi_n = \sqrt{n+1}\Psi_{n+1} \tag{29}$$

and

$$\hat{\Omega}\Psi_n = \Omega(E_n)\Psi_n = (E_{n+1} - E_n)\Psi_n \tag{30}$$

if the operators $\hat{b}$ and $\hat{\Omega}$ are given by equation (27). In the particular case of the dimensionless anharmonic oscillators

$$\hat{H} = \tfrac{1}{2}(\hat{p}^2 + \hat{x}^2) + \lambda \hat{x}^{2K} \qquad K = 2, 3, \ldots \tag{31}$$

where $[\hat{x}, \hat{p}] = i$, the coefficients of the series (16) for the frequency operator are polynomial functions of the Hamiltonian operator:

$$\Omega(\hat{H}) = \sum_{i=0}^{\infty} \lambda^i \sum_{j=0}^{(K-1)i} d_{ji} \hat{H}^j. \tag{32}$$

Therefore, if we substitute the well-known Rayleigh–Schrödinger perturbation series (19) into $\Omega(E_n) - E_{n+1} + E_n = 0$, we easily obtain the coefficients d_{ji} of the expansion (32).

We have calculated the Rayleigh–Schrödinger perturbation series for the energy in terms of $E_{n,0} = \epsilon_n$ by means of the method of Swenson and Danforth [3] and the assistance of the computer algebra system Maple (Maple 7, Waterloo Maple Inc., 2000). In this way we easily obtain

$$\begin{aligned}
\Omega^{K=2}(\hat{H}) &= 1 + \left(\tfrac{3}{2} + 3\hat{H}\right)\lambda - \left(\tfrac{153}{16} + \tfrac{51}{4}\hat{H} + \tfrac{69}{4}\hat{H}^2\right)\lambda^2 + \left(\tfrac{1305}{16} + \tfrac{3615}{16}\hat{H}\right. \\
&\quad \left. + \tfrac{639}{4}\hat{H}^2 + \tfrac{633}{4}\hat{H}^3\right)\lambda^3 + \cdots \\
\Omega^{K=3}(\hat{H}) &= 1 + \left(\tfrac{45}{8} + \tfrac{15}{2}\hat{H} + \tfrac{15}{2}\hat{H}^2\right)\lambda - \left(\tfrac{58\,725}{256} + \tfrac{17\,115}{32}\hat{H} + \tfrac{21\,795}{32}\hat{H}^2 + \tfrac{2115}{8}\hat{H}^3\right. \\
&\quad \left. + \tfrac{2565}{16}\hat{H}^4\right)\lambda^2 + \tfrac{53\,895\,375}{2048} + \tfrac{19\,803\,855}{256}\hat{H} + \tfrac{59\,204\,895}{512}\hat{H}^2 \\
&\quad + \tfrac{2509\,125}{32}\hat{H}^3 + \tfrac{6670\,125}{128}\hat{H}^4 + \tfrac{189\,495}{16}\hat{H}^5 + \tfrac{164\,805}{32}\hat{H}^6\Big)\lambda^3 + \cdots \\
\Omega^{K=4}(\hat{H}) &= 1 + \left(\tfrac{315}{16} + \tfrac{385}{8}\hat{H} + \tfrac{105}{4}\hat{H}^2 + \tfrac{35}{2}\hat{H}^3\right)\lambda - \left(\tfrac{21\,575\,925}{2048} + \tfrac{14\,152\,075}{512}\hat{H}\right. \\
&\quad + \tfrac{20\,218\,835}{512}\hat{H}^2 + \tfrac{1529\,605}{64}\hat{H}^3 + \tfrac{1886\,955}{128}\hat{H}^4 + \tfrac{91\,035}{32}\hat{H}^5 \\
&\quad \left. + \tfrac{35\,245}{32}\hat{H}^6\right)\lambda^2 + \tfrac{2519\,391\,160\,125}{131\,072} + \tfrac{4427\,902\,688\,545}{65\,536}\hat{H} \\
&\quad + \tfrac{799\,555\,246\,385}{8192}\hat{H}^2 + \tfrac{413\,550\,044\,985}{4096}\hat{H}^3 + \tfrac{234\,829\,791\,035}{4096}\hat{H}^4 \\
&\quad + \tfrac{65\,083\,588\,255}{2048}\hat{H}^5 + \tfrac{4469\,666\,565}{512}\hat{H}^6 + \tfrac{812\,317\,765}{256}\hat{H}^7 + \tfrac{189\,065\,205}{512}\hat{H}^8 \\
&\quad + \tfrac{25\,941\,545}{256}\hat{H}^9\Big)\lambda^3 + \cdots
\end{aligned} \tag{33}$$

for the quartic ($K = 2$), sextic ($K = 3$) and octic ($K = 4$) oscillators, respectively. This equation extends Speliotopoulos' second-order result for $K = 2$ (18) [16] to third order, and shows two other cases $K = 3$ and $K = 4$ that were not published before, as far as we know. Proceeding as already indicated above, we can easily derive similar expressions for any other anharmonic oscillator as well as for higher perturbation orders.

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