

Multiple-Scale Analysis of the Quantum Anharmonic Oscillator

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Conventional weak-coupling perturbation theory suffers from problems that arise from the resonant coupling of successive orders in the perturbation series. Multiple-scale perturbation theory avoids such problems by implicitly performing an infinite reordering and resummation of the conventional perturbation series. Multiple-scale analysis provides a good description of the *classical* anharmonic oscillator. Here, it is extended to study the Heisenberg operator equations of motion for the quantum anharmonic oscillator. The analysis yields a system of nonlinear operator differential equations, which is solved exactly. The solution provides an operator mass renormalization of the theory. [S0031-9007(96)01684-5]

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Multiple-scale perturbation theory (MSPT) is a powerful and sophisticated perturbative method for solving physical problems having a small parameter ϵ [1,2]. MSPT is applicable to both linear and nonlinear problems. Indeed, it is so general that other perturbative methods such as WKB theory and boundary-layer theory, which are useful in more limited contexts, may be viewed as special cases of MSPT [1].

MSPT recognizes that dynamical systems exhibit characteristic physical behaviors at various length or time scales. The problem with conventional perturbation theory is that there is often a resonant coupling between successive orders. This coupling gives rise to *secular terms* (terms that grow rapidly with the length or time variable) in the perturbation series. Secular terms conflict with physical requirements that the solution be finite. MSPT *reorganizes* the conventional perturbation series to eliminate secular terms, and, in doing so, it describes quantitatively the behaviors that occur at many scales.

Ordinarily, MSPT is applied to *classical* differential equations such as Duffing's equation (the nonlinear equation of motion for the classical anharmonic oscillator):

$$y'' + y + 4\epsilon y^3 = 0 \quad (\epsilon \geq 0). \quad (1)$$

The positivity of ϵ ensures that $y(t)$ is bounded [1]. The classical harmonic oscillator ($\epsilon = 0$) has only one time scale, the period of oscillation. However, when $\epsilon \neq 0$, the nonlinear term in Eq. (1) introduces many time scales. Using MSPT, one can show that on a long-time scale [$t = O(\epsilon^{-1})$] there is a frequency shift of order ϵ .

In this Letter we generalize MSPT and apply it to the Heisenberg operator equations of motion of the *quantum* anharmonic oscillator (the quantum version of Duffing's equation). This generalization of MSPT techniques is nontrivial because it gives rise to a nonlinear system of *operator* differential equations [3]. We find the exact closed-form solution to this system and thereby obtain the quantum operator analog of the classical frequency shift—an *operator mass renormalization* that expresses the first-order shift of all energy levels.

We begin our presentation by reviewing the difficulties one encounters when one tries to solve Duffing's equation using a conventional perturbation series, $y(t) = \sum_{n=0}^{\infty} \epsilon^n y_n(t)$. We choose as initial conditions

$$y(0) = 1 \quad \text{and} \quad y'(0) = 0, \quad (2)$$

which translate into $y_n(0) = \delta_{n,0}$ and $y'_n(0) = 0$, and substitute $y(t)$ into Eq. (1). To zeroth and first order in powers of ϵ , we have

$$y_0'' + y_0 = 0, \quad (3)$$

$$y_1'' + y_1 = -4y_0^3. \quad (4)$$

The solution to Eq. (3) satisfying the initial conditions is $y_0(t) = \cos t$. Introducing this solution into Eq. (4), we obtain $y_1'' + y_1 = -\cos(3t) - 3\cos t$, which represents a forced harmonic oscillator whose driving term has frequencies 3 and 1. A harmonic oscillator when driven at its natural frequency, which in this case is 1, exhibits resonance. As a result, the solution $y_1(t) = \frac{1}{8}\cos(3t) - \frac{1}{8}\cos t - \frac{3}{2}t\sin t$ contains a secular term that grows linearly with time t . The function $y_1(t)$ cannot be valid for long times because the exact solution to Duffing's equation remains bounded for all t [1]. Hence, the conventional perturbation expansion is sensible only for short times $t \ll \epsilon^{-1}$.

If one is clever, one can use the conventional perturbation series to determine $y(t)$ for long times, say, of order ϵ^{-1} . To do so, we note [1] that the structure of the most secular (highest power in t) term in $y_n(t)$ has the form $\frac{1}{2}(3it/2)^n e^{it}/n! + \text{c.c.}$; we then approximate $y(t)$ by summing the most secular term in every order, and the result is a cosine function that remains bounded for all times t :

$$\frac{1}{2} \sum_{n=0}^{\infty} \left[\left(\frac{3i\epsilon t}{2} \right)^n \frac{e^{it}}{n!} + \text{c.c.} \right] = \cos \left[\left(1 + \frac{3}{2}\epsilon \right) t \right]. \quad (5)$$

Hence, on the long-time scale $\tau = \epsilon t$, we see a *frequency shift* in the oscillator of order $\frac{3}{2}\epsilon$. This result is not exact

because there are less secular terms to all orders in the perturbation expansion; such terms give rise to frequency shifts of order $\epsilon^2, \epsilon^3, \dots$.

The advantage of MSPT is that it reproduces Eq. (5) directly and bypasses the elaborate procedure of summing the conventional perturbation series to all orders by excluding *ab initio* secular terms from the perturbation expansion. MSPT assumes the existence of many time scales ($t, \tau = \epsilon t, \sigma = \epsilon^2 t, \dots$), which can be temporarily treated as *independent* variables. Here, we illustrate by performing just a first-order calculation. We use only the two variables t and $\tau = \epsilon t$, and seek a perturbative solution to Eq. (1) of the form,

$$y(t) = Y_0(t, \tau) + \epsilon Y_1(t, \tau) + O(\epsilon^2). \quad (6)$$

The chain rule and the identity $\frac{d\tau}{dt} = \epsilon$ convert Eq. (1) to a sequence of *partial* differential equations for the dependent variables Y_0, Y_1, \dots . The first two are

$$\frac{\partial^2}{\partial t^2} Y_0 + Y_0 = 0, \quad (7)$$

$$\frac{\partial^2}{\partial t^2} Y_1 + Y_1 = -4Y_0^3 - 2\frac{\partial^2}{\partial t \partial \tau} Y_0. \quad (8)$$

The general solution to Eq. (7) is $Y_0(t, \tau) = A(\tau) \cos t + B(\tau) \sin t$. We substitute $Y_0(t, \tau)$ into the right side of Eq. (8) and use triple-angle formulas such as $\cos^3 t = \frac{1}{4} \cos(3t) + \frac{3}{4} \cos t$ to simplify the result. To determine the functions $A(\tau)$ and $B(\tau)$ we demand that there be no resonant coupling between zeroth and first order in perturbation theory so that no secular terms appear in Y_1 . That is, we require that the coefficients of $\sin t$ and $\cos t$ vanish:

$$2\frac{dB}{d\tau} = -3A^3 - 3AB^2 \quad \text{and} \quad 2\frac{dA}{d\tau} = 3B^3 + 3A^2B. \quad (9)$$

To solve this system we multiply the first equation by $B(\tau)$, the second by $A(\tau)$, and add the resulting equations. Letting $C(\tau) = \frac{1}{2}[A(\tau)]^2 + \frac{1}{2}[B(\tau)]^2$, we obtain

$$\frac{d}{d\tau} C(\tau) = 0. \quad (10)$$

Thus, $C(\tau)$ is the constant $C(0)$, and the differential equation system (9) becomes linear:

$$\frac{d}{d\tau} B = -3C(0)A \quad \text{and} \quad \frac{d}{d\tau} A = 3C(0)B. \quad (11)$$

The solution to this system that satisfies the initial conditions is $C(0) = \frac{1}{2}$ and $Y_0(t, \tau) = \cos[(1 + \frac{3}{2}\epsilon)t]$, which reproduces the approximate solution in Eq. (5). While conventional perturbation theory is valid for $t \ll \epsilon^{-1}$, the MSPT approximation is valid for $t \ll \epsilon^{-2}$.

We now consider the *quantum* anharmonic oscillator, whose Hamiltonian is $H(p, q) = \frac{1}{2}p^2 + \frac{1}{2}q^2 + \epsilon q^4$. Here, $\epsilon \geq 0$ so that the spectrum of $H(p, q)$ is bounded below, and p and q are operators [4] satisfying the canonical equal-time commutation relation $[q(t), p(t)] = i\hbar$.

The Heisenberg operator equations of motion, $\frac{d}{dt} q = \frac{1}{i\hbar}[q, H(p, q)] = p$ and $\frac{d}{dt} p = \frac{1}{i\hbar}[p, H(p, q)] =$

$-q - 4\epsilon q^3$, combine to give the quantum Duffing's equation (1):

$$\frac{d^2}{dt^2} q + q + 4\epsilon q^3 = 0. \quad (12)$$

Since $p(t)$ and $q(t)$ are operators, we cannot impose numerical initial conditions such as those in Eq. (2); rather, we enforce a general operator initial condition at $t = 0$:

$$q(0) = q_0 \quad \text{and} \quad p(0) = p_0, \quad (13)$$

where p_0 and q_0 are time-independent operators obeying the Heisenberg algebra $[q_0, p_0] = i\hbar$.

We now apply MSPT to Eq. (12). Assuming that $q(t)$ exhibits characteristic behavior on the short-time scale t , and, on the long-time scale $\tau = \epsilon t$, we write

$$q(t) = Q(t, \tau) = Q_0(t, \tau) + \epsilon Q_1(t, \tau) + O(\epsilon^2). \quad (14)$$

This equation is analogous to Eq. (6), but here Q_0 and Q_1 are *operator-valued* functions.

We substitute $q(t)$ in Eq. (14) into Eq. (12), collect the coefficients of ϵ^0 and ϵ^1 , and obtain operator differential equations analogous to Eqs. (7) and (8):

$$\frac{\partial^2}{\partial t^2} Q_0 + Q_0 = 0, \quad (15)$$

$$\frac{\partial^2}{\partial t^2} Q_1 + Q_1 = -4Q_0^3 - 2\frac{\partial^2}{\partial t \partial \tau} Q_0. \quad (16)$$

Because Eq. (15) is linear, it is easy to find its general solution,

$$Q_0(t, \tau) = \mathcal{A}(\tau) \cos t + \mathcal{B}(\tau) \sin t, \quad (17)$$

and from $p = \frac{dq}{dt}$ we obtain the momentum operator $p(t) = \mathcal{B}(\tau) \cos t - \mathcal{A}(\tau) \sin t + O(\epsilon)$.

It is now necessary to find the coefficient functions $\mathcal{A}(\tau)$ and $\mathcal{B}(\tau)$, which are operators. The canonical commutation relation $[q(t), p(t)] = i\hbar$ implies that these operators satisfy $[\mathcal{A}(\tau), \mathcal{B}(\tau)] = i\hbar$. Also, the initial conditions in Eq. (13) give

$$\mathcal{A}(0) = q_0 \quad \text{and} \quad \mathcal{B}(0) = p_0. \quad (18)$$

We determine $\mathcal{A}(\tau)$ and $\mathcal{B}(\tau)$ by evaluating the right side of Eq. (16) and expanding the cubic term, taking care to preserve the order of operator multiplication. As in the classical case, we simplify the result using triple-angle formulas. To prevent secularities in $Q_1(t, \tau)$ we set the coefficients of $\cos t$ and $\sin t$ to zero and obtain

$$\begin{aligned} 2\frac{d\mathcal{B}}{d\tau} &= -3\mathcal{A}^3 - \mathcal{B}\mathcal{A}\mathcal{B} - \mathcal{B}\mathcal{B}\mathcal{A} - \mathcal{A}\mathcal{B}\mathcal{B}, \\ 2\frac{d\mathcal{A}}{d\tau} &= 3\mathcal{B}^3 + \mathcal{A}\mathcal{B}\mathcal{A} + \mathcal{A}\mathcal{A}\mathcal{B} + \mathcal{B}\mathcal{A}\mathcal{A}. \end{aligned} \quad (19)$$

This system of operator-valued differential equations is the quantum analog of Eq. (9).

To solve the system (19) we premultiply and postmultiply the first equation by $\mathcal{B}(\tau)$ and the second equation by

$\mathcal{A}(\tau)$. Adding the resulting four equations, we get

$$\frac{d}{d\tau}\mathcal{H} = 0, \quad (20)$$

where $\mathcal{H} \equiv \frac{1}{2}\mathcal{A}^2 + \frac{1}{2}\mathcal{B}^2$. Equation (20), the quantum analog of Eq. (10), shows that \mathcal{H} is independent of the long-time variable τ . Thus, Eq. (18) allows us to express \mathcal{H} in terms of the fundamental operators p_0 and q_0 : $\mathcal{H} = \frac{1}{2}p_0^2 + \frac{1}{2}q_0^2$. We then use the commutator $[\mathcal{A}(\tau), \mathcal{B}(\tau)] = i\hbar$ to rewrite Eq. (19) in manifestly Hermitian form:

$$\begin{aligned} \frac{d}{d\tau}\mathcal{B} &= -\frac{3}{2}(\mathcal{H}\mathcal{A} + \mathcal{A}\mathcal{H}), \\ \frac{d}{d\tau}\mathcal{A} &= \frac{3}{2}(\mathcal{H}\mathcal{B} + \mathcal{B}\mathcal{H}). \end{aligned} \quad (21)$$

Suppose for a moment that we could replace the operator \mathcal{H} by the numerical constant $C(0)$ in Eq. (21). Then we would obtain the c -number coupled differential equations in Eq. (11). That system is linear, so we could ignore operator ordering and easily find the solution satisfying the initial conditions (18): $\mathcal{A}(\tau) = q_0 \cos[3C(0)\tau] + p_0 \sin[3C(0)\tau]$ and $\mathcal{B}(\tau) = p_0 \cos[3C(0)\tau] - q_0 \sin[3C(0)\tau]$. This solution suggests the structure of the exact solution to the operator differential equation system (21). The formal solution is a natural generalization using Weyl-ordered products of operators:

$$\begin{aligned} \mathcal{A}(\tau) &= \mathcal{W}[q_0 \cos(3\mathcal{H}\tau) + p_0 \sin(3\mathcal{H}\tau)], \\ \mathcal{B}(\tau) &= \mathcal{W}[p_0 \cos(3\mathcal{H}\tau) - q_0 \sin(3\mathcal{H}\tau)]. \end{aligned} \quad (22)$$

The operator ordering $\mathcal{W}[q_0 f(\mathcal{H}\tau)]$ is defined as follows: (1) Expand $f(\mathcal{H}\tau)$ as a Taylor series in powers of the operator $\mathcal{H}\tau$; (2) Weyl order the Taylor series term by term: $\mathcal{W}(q_0 \mathcal{H}^n) \equiv \frac{1}{2^n} \sum_{j=0}^n \binom{n}{j} \mathcal{H}^j q_0 \mathcal{H}^{n-j}$. Using this definition it is easy to verify that Eq. (22) is indeed the *exact operator solution* to Eq. (21), satisfying the initial conditions (18). We simplify the formal solution in Eq. (22) and reexpress it in closed form by observing that, if we reorder $\mathcal{W}(q_0 \mathcal{H}^n)$ by commuting q_0 symmetrically to the left and to the right to maintain the Hermitian form, we generate a set of polynomials [5] of degree n :

$$\begin{aligned} \mathcal{W}(q_0 \mathcal{H}^n) &= \frac{\hbar^n}{2} \left[q_0 E_n \left(\frac{\mathcal{H}}{\hbar} + \frac{1}{2} \right) \right. \\ &\quad \left. + E_n \left(\frac{\mathcal{H}}{\hbar} + \frac{1}{2} \right) q_0 \right]. \end{aligned}$$

We identify E_n as the n th Euler polynomial [6] in which the argument is shifted by $\frac{1}{2}$:

$$\begin{aligned} 1, \frac{\mathcal{H}}{\hbar}, \frac{\mathcal{H}^2}{\hbar^2} - \frac{1}{4}, \frac{\mathcal{H}^3}{\hbar^3} - \frac{3}{4} \frac{\mathcal{H}}{\hbar}, \\ \frac{\mathcal{H}^4}{\hbar^4} - \frac{3}{2} \frac{\mathcal{H}^2}{\hbar^2} + \frac{5}{16}, \end{aligned}$$

and so on. The generating function for these nonorthogonal polynomials is

$$\frac{2e^{(\mathcal{H}/\hbar+1/2)\tau}}{e^\tau + 1} = \sum_{n=0}^{\infty} \frac{\tau^n}{n!} E_n \left(\frac{\mathcal{H}}{\hbar} + \frac{1}{2} \right) \quad (|\tau| < \pi).$$

This generating function allows us to express the following Weyl-ordered product compactly:

$$\mathcal{W}(q_0 e^{\mathcal{H}\tau}) = \frac{q_0 e^{\mathcal{H}\tau} + e^{\mathcal{H}\tau} q_0}{2 \cosh(\tau\hbar/2)}. \quad (23)$$

Using Eq. (23) we rewrite compactly the cosines and sines in Eq. (22), substitute this result into Eq. (17), replace τ by ϵt , and obtain

$$\begin{aligned} Q_0(t, \tau) &= \frac{q_0 \cos(t + 3\mathcal{H}\epsilon t) + \cos(t + 3\mathcal{H}\epsilon t) q_0}{2 \cos(3\epsilon t\hbar/2)} \\ &\quad + \frac{p_0 \sin(t + 3\mathcal{H}\epsilon t) + \sin(t + 3\mathcal{H}\epsilon t) p_0}{2 \cos(3\epsilon t\hbar/2)}. \end{aligned} \quad (24)$$

Equation (24) is the quantum operator analog of Eq. (5) and is the objective of our multiscale analysis. [We can recover the classical MSPT approximation in Eq. (5) by taking the limit $\hbar \rightarrow 0$ and imposing the classical initial conditions $p_0 = 0$ and $q_0 = 1$, which give $\mathcal{H} = \frac{1}{2}$.] Recall that in the classical case we identify the coefficient of the time t as a first-order approximation to the frequency shift. Since the coefficient of t in Eq. (24) is an operator, we have derived an *operator form of mass renormalization*.

To elucidate this operator mass renormalization we study matrix elements of Eq. (24). The time dependence of a matrix element reveals the energy-level differences of the quantum system. It is easy to construct a set of states because the operators q_0 and p_0 satisfy the Heisenberg algebra $[q_0, p_0] = i\hbar$. Hence, appropriate linear combinations of q_0 and p_0 may be used as raising and lowering operators to generate a Fock space consisting of the states $|n\rangle$. By construction, these states are eigenstates of the operator \mathcal{H} : $\mathcal{H}|n\rangle = (n + \frac{1}{2})\hbar|n\rangle$. Evaluating Eq. (24) between the states $\langle n-1|$ and $|n\rangle$, and allowing the operator \mathcal{H} to act to the left and the right, we obtain

$$\begin{aligned} \langle n-1|Q_0|n\rangle &= \langle n-1|q_0|n\rangle \cos[t(1 + 3n\hbar\epsilon)] \\ &\quad + \langle n-1|p_0|n\rangle \sin[t(1 + 3n\hbar\epsilon)], \end{aligned} \quad (25)$$

which predicts that the energy-level differences of the quantum oscillator are $1 + 3n\hbar\epsilon$. We may verify this result by recalling that the first-order correction to the energy eigenvalues [7] is $E_n = n + \frac{1}{2} + \frac{3}{4}\epsilon\hbar(2n^2 + 2n + 1) + O(\epsilon^2)$. Thus, $E_n - E_{n-1} = 1 + 3n\hbar\epsilon + O(\epsilon^2)$.

We conclude by noting that, in addition to the operators $q(t)$ and $p(t)$, the wave function $\psi(x)$ for the quantum anharmonic oscillator also exhibits multiscale behavior. Specifically, to all orders in conventional weak-coupling Rayleigh-Schrödinger perturbation theory, $\psi(x)$ behaves the same as the Gaussian $e^{-x^2/4}$ for large x ; however, a geometrical-optics approximation to $\psi(x)$ from WKB theory predicts that, for large x , $\psi(x)$ decays the same as

the exponential of a cubic $e^{-\sqrt{\epsilon}|x|^3/6}$. We can resolve this discrepancy by using a MSPT approach; we reorder the perturbation series by resumming secular terms [8].

The wave function $\psi(x)$ obeys the Schrödinger equation,

$$\left(-\frac{d^2}{dx^2} + \frac{1}{4}x^2 + \frac{1}{4}\epsilon x^4 - E(\epsilon)\right)\psi(x) = 0, \quad (26)$$

and satisfies $\psi(\pm\infty) = 0$. The conventional perturbative approach to Eq. (26) [7] represents both the eigenfunction and eigenvalue as asymptotic series in ϵ : $\psi(x) \sim \sum_{n=0}^{\infty} \epsilon^n y_n(x)$ and $E(\epsilon) \sim \sum_{n=0}^{\infty} \epsilon^n E_n$. In Ref. [7] it is shown that, for the ground state, $y_n(x)$ is a Gaussian multiplied by a polynomial of degree $2n$ in the variable x^2 , $y_n = e^{-x^2/4} P_n(x)$, where

$$P_0(x) = 1 \quad \text{and} \quad P_n(x) = \sum_{j=1}^{2n} C_{n,k} \left(-\frac{1}{2}x^2\right)^k (n > 0).$$

The recursion relation for the polynomials $P_n(x)$ is typical of all perturbative calculations; the homogeneous part of this recursion relation is independent of n while the inhomogeneous part contains all previous polynomials. This recursive structure is responsible for successive orders of perturbation theory being resonantly coupled and causes the degree of the polynomials to grow with n .

To study the behavior of the wave function $\psi(x)$ for large x , we approximate $\psi(x)$ by resumming the perturbation series and keeping just the *highest power* of x in every order. [This is an exact analog of finding the coefficient of the highest power of t (most secular term) in n th order in perturbation theory for the classical anharmonic oscillator.] This resummation gives a new representation of $\psi(x)$: $e^{-x^2/4} e^{-\epsilon x^4/16}$ multiplied by a *new set of polynomials*. For the classical anharmonic oscillator, summing leading secular terms also gives an exponential approximation [see Eq. (5)]. However, the classical and quantum anharmonic oscillators are quite different; although we have summed the most secular terms to all orders in perturbation theory, the result is *not* the actual behavior of the wave function $\psi(x)$ for large x ; the correct behavior is an exponential of a cubic and not a quartic.

If we iterate this resummation process we find that each reorganization of the perturbation series gives an additional term in the exponential

$$\exp\left(-\frac{1}{4}x^2 - \frac{1}{16}\epsilon x^4 + \frac{1}{96}\epsilon^2 x^6 - \frac{1}{256}\epsilon^3 x^8 + \dots\right) \quad (27)$$

and a new set of polynomials. It seems impossible for this approach to give cubic exponential behavior because, at each stage in the reorganization of the perturbation series, the variable x appears only in *even* powers. However, we recognize that the exponent in Eq. (27) is the beginning of a binomial series whose sum is $\frac{1}{6\epsilon}[1 - (1 + \epsilon x^2)^{3/2}]$. If we now let x be large ($\epsilon x^2 \gg 1$), we recover the correct asymptotic behavior of $\psi(x)$ [9].

The approach used above for the anharmonic oscillator wave function has been used in perturbative quantum field theory to sum leading-logarithm divergences [10] and leading infrared divergences [11]. It is our hope that in the future the direct nonperturbative multivariate approach of MSPT will provide a framework to simplify such schemes.

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