Multiple-scale analysis of quantum systems

Carl M. Bender* and Luís M. A. Bettencourt
Blackett Laboratory, Imperial College, London SW7 2BZ, United Kingdom
(Received 9 July 1996)

Conventional weak-coupling Rayleigh-Schrödinger perturbation theory suffers from problems that arise from resonant coupling of successive orders in the perturbation series. Multiple-scale analysis, a powerful and sophisticated perturbative method that quantitatively analyzes characteristic physical behaviors occurring on various length or time scales, avoids such problems by implicitly performing an infinite resummation of the conventional perturbation series. Multiple-scale perturbation theory provides a good description of the classical anharmonic oscillator. Here, it is extended to study (1) the Heisenberg operator equations of motion and (2) the Schrödinger equation for the quantum anharmonic oscillator. In the former case, it leads to a system of coupled operator differential equations, which is solved exactly. The solution provides an operator mass renormalization of the theory. In the latter case, multiple-scale analysis elucidates the connection between weak-coupling perturbative and semiclassical nonperturbative aspects of the wave function. [S0556-2821(96)00324-4]

PACS number(s): 11.15.Bt, 02.30.Mv, 11.15.Tk

I. INTRODUCTION

Multiple-scale perturbation theory (MSPT) is a powerful and sophisticated perturbative technique for solving physical problems having a small parameter ϵ [1–3]. This perturbation method is generally useful for both linear and nonlinear problems. In fact, it is so general that other well-known 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].

The key idea underlying MSPT is that dynamical systems tend to exhibit distinct characteristic physical behaviors at different length or time scales. If a conventional perturbation series is used to solve a problem, then there is often a resonant coupling between successive orders of perturbation theory. This coupling gives rise to *secular terms* in the perturbation series (terms that grow rapidly as functions of the length or time variable). These secular terms conflict with physical requirements that the solution be finite. MSPT *reorganizes* the perturbation series to eliminate secular growth, and in doing so it gives a quantitative description of the characteristic behaviors that occur at many scales. In the past MSPT has been used to solve *classical* differential equations such as the equation of motion for the classical anharmonic oscillator. Indeed, the classical anharmonic oscillator is often used to illustrate and explain the method of MSPT.

In this paper we generalize the ideas of MSPT to the *quantum* anharmonic oscillator [4]. The quantum anharmonic oscillator is an excellent laboratory for the study of a variety of perturbative methods. It has been used to study the origin of the divergence of conventional weak-coupling Rayleigh-Schrödinger perturbation theory [5], Padé and Borel summation of perturbation series [6], large-order behavior of perturbation theory [7], δ expansions [8], dimensional expansions [9], and strong-coupling expansions [10]. Here, we use MSPT to study two aspects of the quantum anharmonic oscillator, the Heisenberg operator equations of motion in Secs. II and III and the Schrödinger equation in Secs. IV and V. We illustrate the methods of MSPT in Sec. II by applying it to the nonlinear dynamical equation of motion for the classical anharmonic oscillator (Duffing's equation). There, we obtain the first-order frequency shift. Then, in Sec. III we extend the methods of MSPT to the nonlinear Heisenberg equation for the quantum anharmonic oscillator (the quantum version of Duffing's equation). To complete the analysis it is necessary to solve a nonlinear system of coupled operator differential equations. We find the exact closed-form solution to this system. From this solution, we obtain the quantum operator analogue of the frequency shift; namely, an operator mass renormalization that expresses the first-order shift of all energy levels.

In the next two sections we study the Schrödinger equation for the quantum anharmonic oscillator. Specifically, we examine the asymptotic behavior of the wave function $\psi(x)$ for large x. We consider the problem of reconciling the different results that one obtains from conventional Rayleigh-Schrödinger perturbation theory (a formal Taylor series in powers of a small parameter ϵ) and WKB theory (a nonperturbative probe of the anharmonic oscillator that is valid regardless of the size of ϵ). To any finite order in conventional perturbation theory, $\psi(x)$ behaves like a Gaussian for large x; however, WKB theory predicts that as $x \to \infty$ the wave function decays to zero like the exponential of a cubic. In Sec. IV we resolve this discrepancy at two different length scales by an infinite sequence of reorderings and resummations of the conventional weak-coupling perturbation series. In Sec. V we explain the origin of the disparity by performing a direct multiple-scale analysis of the Schrödinger equation for the quantum anharmonic oscillator.

The approach used in this paper for the anharmonic oscillator wave function has been applied in perturbative quantum field theory to sum leading-logarithm divergences [11] and leading infrared divergences [12]. It is our hope that in the future the direct nonperturbative multivariate approach of MSPT will provide a framework to simplify such schemes.

*Permanent address: Department of Physics, Washington University, St. Louis, MO 63130.

II. MULTIPLE-SCALE PERTURBATION THEORY APPLIED TO THE CLASSICAL ANHARMONIC OSCILLATOR

In this section we explain MSPT by using it to treat the classical anharmonic oscillator, a dynamical system satisfying the nonlinear differential equation

$$\frac{d^2}{dt^2}y+y+4\epsilon y^3=0 \quad (\epsilon>0), \tag{2.1}$$

which is known as Duffing's equation. The positivity of ϵ ensures that there are no unbounded runaway modes. We impose the initial conditions

$$y(0)=1 \quad \text{and} \quad y'(0)=0. \tag{2.2}$$

The harmonic oscillator ($\epsilon=0$) has only one time scale, namely, the period of oscillation. However, the nonlinear term in Eq. (2.1) introduces many time scales into the problem. For example, when $\epsilon\neq 0$, one can observe on a long-time scale [$t=O(\epsilon^{-1})$] a frequency shift of order ϵ. One can study the classical anharmonic oscillator on the short-time scale t and also on many long-time scales $\tau=\epsilon t$, $\tau_1=\epsilon^2 t$, $\tau_2=\epsilon^3 t$, and so on.

Let us first examine what happens if we attempt to solve Duffing's equation using a conventional perturbation series in powers of the parameter ϵ,

$$y(t)=\sum_{n=0}^{\infty}\epsilon^n y_n(t), \tag{2.3}$$

in which the initial conditions in Eq. (2.2) are contained as

$$y_0(0)=1 \quad \text{and} \quad y_0'(0)=0,$$

$$y_n(0)=y_n'(0)=0 \quad (n\geq 1). \tag{2.4}$$

Substitute Eq. (2.3) into Eq. (2.1). To leading order (zeroth order in powers of ϵ), we have

$$\frac{d^2}{dt^2}y_0+y_0=0 \tag{2.5}$$

and to first order in powers of ϵ we have

$$\frac{d^2}{dt^2}y_1+y_1=-4y_0^3. \tag{2.6}$$

The solution to Eq. (2.5) satisfying the initial conditions in Eq. (2.4) is

$$y_0(t)=\cos t. \tag{2.7}$$

When we introduce this solution into Eq. (2.6), we obtain

$$\frac{d^2}{dt^2}y_1+y_1=-\cos(3t)-3\cos t. \tag{2.8}$$

Equation (2.8) represents a forced harmonic oscillator whose driving term has frequencies 3 and 1. When a harmonic oscillator is driven at its natural frequency, which in this case is 1, we have the phenomenon of resonance. As a result, the solution

$$y_1(t)=\frac{1}{8}\cos(3t)-\frac{1}{8}\cos t-\frac{3}{2}t\sin t \tag{2.9}$$

contains a secular term that grows linearly with increasing time t. Equation (2.9) 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 $t\ll\epsilon^{-1}$. How then does the conventional perturbation series determine the behavior of $y(t)$ for long times, say of order ϵ^{-1}?

One way to answer this question is to identify the structure of the most secular (highest power in t) term *to all orders* in perturbation theory. One can easily verify [1] that for all n the most secular term in $y_n(t)$ has the form

$$\frac{1}{2}\frac{t^n}{n!}\left[\left(\frac{3i}{2}\right)^n e^{it}+\left(-\frac{3i}{2}\right)^n e^{-it}\right]. \tag{2.10}$$

Since the expression in Eq. (2.10) is multiplied by ϵ^n, if we make the approximation of retaining only the most secular term in every order, then we obtain a series in powers of the long-time variable $\tau=\epsilon t$. Evidently, we can sum the most secular terms in this series to all orders in ϵ, and since the result is a cosine function, it remains bounded for all times t:

$$\frac{1}{2}\sum_{n=0}^{\infty}\frac{\epsilon^n t^n}{n!}\left[\left(\frac{3i}{2}\right)^n e^{it}+\left(-\frac{3i}{2}\right)^n e^{-it}\right]=\cos\left[\left(1+\frac{3}{2}\epsilon\right)t\right]. \tag{2.11}$$

We interpret this result to mean that on the long-time scale τ there is a *frequency shift* in the oscillator of order $\frac{3}{2}\epsilon$. Of course, this result is not exact; there are less secular terms to all orders in the perturbation expansion, and these terms give rise to frequency shifts of order ϵ^2, ϵ^3, and so on.

We will now show how MSPT directly reproduces the result in Eq. (2.11). To avoid the complicated procedure of summing the conventional perturbation series to all orders in powers of ϵ, MSPT uses a sophisticated perturbative approach that prevents secular terms from appearing in the perturbation expansion. Multiple-scale analysis assumes *a priori* the existence of many time scales $(t,\tau,\tau_1,\tau_2,\ldots)$ in the problem, 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. (2.1) of the form

$$y(t)=Y_0(t,\tau)+\epsilon Y_1(t,\tau)+O(\epsilon^2). \tag{2.12}$$

Using the chain rule and the identity $\partial\tau/\partial t=\epsilon$, we convert Eq. (2.1) to a sequence of *partial* differential equations for the dependent variables Y_0, Y_1, ... The first two equations read

$$\frac{\partial^2}{\partial t^2}Y_0+Y_0=0, \tag{2.13}$$

$$\frac{\partial^2}{\partial t^2}Y_1+Y_1=-4Y_0^3-2\frac{\partial^2}{\partial t\partial\tau}Y_0. \tag{2.14}$$

The general solution to Eq. (2.13) is

$$Y_0(t,\tau)=A(\tau)\cos t+B(\tau)\sin t, \tag{2.15}$$

where $A(\tau)$ and $B(\tau)$ are as yet unknown functions of τ. We determine these functions by imposing the condition that no secular terms appear in Y_1. That is, we use the functional freedom in the choice of $A(\tau)$ and $B(\tau)$ to eliminate the resonant coupling between zeroth and first order in perturbation theory. We substitute $Y_0(t,\tau)$ in Eq. (2.15) into the right side of Eq. (2.14) and expand the resulting expression using the trigonometric identities

$$\cos^3 t=\frac{1}{4}\cos(3t)+\frac{3}{4}\cos t,$$

$$\sin^3 t=-\frac{1}{4}\sin(3t)+\frac{3}{4}\sin t,$$

$$\cos^2 t\,\sin t=\frac{1}{4}\sin(3t)+\frac{1}{4}\sin t,$$

$$\sin^2 t\,\cos t=-\frac{1}{4}\cos(3t)+\frac{1}{4}\cos t. \tag{2.16}$$

To eliminate secularity we require that the coefficient of cos*t* and sin*t* vanish. This gives the pair of equations

$$2\frac{dB}{d\tau}=-3A^3-3AB^2$$

and

$$2\frac{dA}{d\tau}=3B^3+3A^2B. \tag{2.17}$$

To solve this system we multiply the first equation by $B(\tau)$ and the second equation by $A(\tau)$. Adding the resulting equations gives

$$\frac{d}{d\tau}C(\tau)=0, \tag{2.18}$$

where

$$C(\tau)=\frac{1}{2}[A(\tau)]^2+\frac{1}{2}[B(\tau)]^2. \tag{2.19}$$

Hence $C(\tau)$ is independent of τ and we may take $C(\tau)=C(0)$.

Substituting this result back into Eq. (2.17) gives the elementary linear system

$$\frac{d}{d\tau}B=-3C(0)A \quad \text{and} \quad \frac{d}{d\tau}A=3C(0)B. \tag{2.20}$$

When we solve this system and then impose the initial conditions, we obtain $C(0)=\frac{1}{2}$ and

$$Y_0(t,\tau)=\cos\left[\left(1+\frac{3}{2}\epsilon\right)t\right], \tag{2.21}$$

where we have used $\tau=\epsilon t$. We have thus reproduced the approximate solution in Eq. (2.11) that is valid for long times. Note that while conventional perturbation theory is only valid for $t\ll\epsilon^{-1}$, the multiple-scale solution is valid for times satisfying $t\ll\epsilon^{-2}$. This multivariate approach can, in principle, be performed to nth order in powers of ϵ for any n.

III. MULTIPLE-SCALE PERTURBATION THEORY APPLIED TO THE QUANTUM ANHARMONIC OSCILLATOR

In this section we extend the multiple-scale approach described in Sec. II to the quantum anharmonic oscillator. This is a nontrivial generalization of the usual multiple-scale techniques because it requires that we solve *operator* differential equations [13].

The quantum anharmonic oscillator is defined by the Hamiltonian [14]

$$H(p,q)=\frac{1}{2}p^2+\frac{1}{2}q^2+\epsilon q^4 \quad (\epsilon>0), \tag{3.1}$$

where p and q are operators satisfying the canonical equal-time commutation relation

$$[q(t),p(t)]=i\hbar. \tag{3.2}$$

The positivity of ϵ ensures that $H(p,q)$ is bounded below.

The Heisenberg operator equations of motion are

$$\frac{d}{dt}q=\frac{1}{i\hbar}[q,H(p,q)]=p, \tag{3.3}$$

$$\frac{d}{dt}p=\frac{1}{i\hbar}[p,H(p,q)]=-q(t)-4\epsilon[q(t)]^3. \tag{3.4}$$

These equations combine to give

$$\frac{d^2}{dt^2}q(t)+q(t)+4\epsilon[q(t)]^3=0, \tag{3.5}$$

which is the quantum analog of Duffing's classical differential equation (2.1). Since $p(t)$ and $q(t)$ are operators, we cannot impose numerical initial conditions like those in Eq. (2.2); rather, we enforce a general operator initial condition at $t=0$:

$$q(0)=q_0 \quad \text{and} \quad p(0)=p_0. \tag{3.6}$$

Here, p_0 and q_0 are fundamental time-independent operators obeying the Heisenberg algebra

$$[q_0,p_0]=i\hbar. \tag{3.7}$$

Rather than seeking a solution to Eq. (3.5) as a conventional perturbation series in powers of ϵ, we perform a multiple-scale analysis. We assume that $q(t)$ exhibits characteristic behavior on the short-time scale t and on the long-time scale $\tau=\epsilon t$ and we write

$$q(t)=Q(t,\tau)=Q_0(t,\tau)+\epsilon Q_1(t,\tau)+O(\epsilon^2). \quad (3.8)$$

This equation is analogous to Eq. (2.12) but here Q_0 and Q_1 are *operator-valued* functions.

There is an associated expression for the momentum operator $p(t)$:

$$p(t)=P_0(t,\tau)+\epsilon P_1(t,\tau)+O(\epsilon^2). \quad (3.9)$$

Furthermore, since the momentum operator is the time derivative of the position operator [see Eq. (3.3)], the chain rule gives

$$p(t)=\frac{\partial}{\partial t}Q_0+\epsilon\left(\frac{\partial}{\partial\tau}Q_0+\frac{\partial}{\partial t}Q_1\right)+O(\epsilon^2). \quad (3.10)$$

We substitute the expression for $q(t)$ in Eq. (3.8) into Eq. (3.5), collect the coefficients of ϵ^0 and ϵ^1, and obtain operator differential equations analogous to Eqs. (2.13) and (2.14):

$$\frac{\partial^2}{\partial t^2}Q_0+Q_0=0, \quad (3.11)$$

$$\frac{\partial^2}{\partial t^2}Q_1+Q_1=-4Q_0^3-2\frac{\partial^2}{\partial t\partial\tau}Q_0. \quad (3.12)$$

Because Eq. (3.11) is linear it is easy to find its general solution:

$$Q_0(t,\tau)=\mathcal{A}(\tau)\cos t+\mathcal{B}(\tau)\sin t, \quad (3.13)$$

from this result we obtain

$$P_0(t,\tau)=\mathcal{B}(\tau)\cos t-\mathcal{A}(\tau)\sin t. \quad (3.14)$$

It is now necessary to find the coefficient functions $\mathcal{A}(\tau)$ and $\mathcal{B}(\tau)$, which are operators. The canonical commutation relations in Eq. (3.2) imply that these operators must satisfy

$$[\mathcal{A}(\tau),\mathcal{B}(\tau)]=i\hbar. \quad (3.15)$$

Also, the initial conditions in Eq. (3.6) give

$$\mathcal{A}(0)=q_0 \quad \text{and} \quad \mathcal{B}(0)=p_0. \quad (3.16)$$

To determine the τ dependence of the functions $\mathcal{A}(\tau)$ and $\mathcal{B}(\tau)$, we must eliminate secular behavior. To do so we examine the right side of Eq. (3.12), which is

$$-4[\mathcal{A}(\tau)\cos t+\mathcal{B}(\tau)\sin t]^3 -2\left[-\frac{d}{d\tau}\mathcal{A}(\tau)\sin t+\frac{d}{d\tau}\mathcal{B}(\tau)\cos t\right]. \quad (3.17)$$

Next, we expand the cubic term, taking care to preserve the order of operator multiplication, and we use the trigonometric identities in Eq. (2.16). We eliminate secularity by setting the coefficients of cos$t$ and sin$t$ to zero and obtain

$$2\frac{d\mathcal{B}}{d\tau}=-3\mathcal{A}^3-\mathcal{B}\mathcal{A}\mathcal{B}-\mathcal{B}\mathcal{B}\mathcal{A}-\mathcal{A}\mathcal{B}\mathcal{B}$$

and

$$2\frac{d\mathcal{A}}{d\tau}=3\mathcal{B}^3+\mathcal{A}\mathcal{B}\mathcal{A}+\mathcal{A}\mathcal{A}\mathcal{B}+\mathcal{B}\mathcal{A}\mathcal{A}. \quad (3.18)$$

This system of operator-valued differential equations is the quantum analog of Eq. (2.17).

To solve the system (3.18) we begin by multiplying the first equation on the left and on the right by $\mathcal{B}(\tau)$ and the second equation on the left and on the right by $\mathcal{A}(\tau)$. Adding the resulting four equations and simplifying, we get

$$\frac{d}{d\tau}\mathcal{H}=0, \quad (3.19)$$

where

$$\mathcal{H}\equiv\frac{1}{2}\mathcal{A}^2+\frac{1}{2}\mathcal{B}^2. \quad (3.20)$$

Equation (3.19) is the quantum analog of $dC/d\tau=0$ in Eq. (2.18). By construction, the operator $\mathcal{H}$ is independent of the short-time variable t. However, Eq. (3.19) shows that $\mathcal{H}$ is also independent of the long-time variable τ. Therefore, Eq. (3.16) allows us to express $\mathcal{H}$ in terms of the fundamental operators p_0 and q_0:

$$\mathcal{H}=\frac{1}{2}p_0^2+\frac{1}{2}q_0^2. \quad (3.21)$$

Next we use Eq. (3.15) to rewrite Eq. (3.18) in manifestly Hermitian form:

$$\frac{d}{d\tau}\mathcal{B}=-\frac{3}{2}(\mathcal{H}\mathcal{A}+\mathcal{A}\mathcal{H})$$

and

$$\frac{d}{d\tau}\mathcal{A}=\frac{3}{2}(\mathcal{H}\mathcal{B}+\mathcal{B}\mathcal{H}). \quad (3.22)$$

Suppose for a moment that we could replace $\mathcal{H}$ by the numerical constant $C(0)$. We would then obtain the elementary classical system of coupled differential equations in Eq. (2.20). Because this system is *linear* we could treat these operator differential equations classically and ignore operator ordering. The solution to this system that satisfies the initial conditions in Eq. (3.16) would then be

$$\mathcal{A}(\tau)=q_0\cos[3C(0)\tau]+p_0\sin[3C(0)\tau]$$

and

$$\mathcal{B}(\tau)=p_0\cos[3C(0)\tau]-q_0\sin[3C(0)\tau]. \quad (3.23)$$

This solution suggests the structure of the exact solution to the *operator* differential equation system (3.22). The formal solution is a natural quantum operator generalization of Eq. (3.23) using Weyl ordered products of operators:

$$\mathcal{A}(\tau)=\mathcal{W}[q_0\cos(3\mathcal{H}\tau)]+\mathcal{W}[p_0\sin(3\mathcal{H}\tau)],$$

$$\mathcal{B}(\tau)=\mathcal{W}[p_0\cos(3\mathcal{H}\tau)]-\mathcal{W}[q_0\sin(3\mathcal{H}\tau)]. \quad (3.24)$$

The notation $\mathcal{W}[q_0 f(\mathcal{H}\tau)]$ represents an operator ordering defined as follows: First, expand the function $f(\mathcal{H}\tau)$ as a Taylor series in powers of the operator $\mathcal{H}\tau$. Then Weyl order the Taylor series term by term:

$$\mathcal{W}(q_0\mathcal{H}^n)\equiv\frac{1}{2^n}[\binom{n}{0}q_0\mathcal{H}^n+\binom{n}{1}\mathcal{H}q_0\mathcal{H}^{n-1}+\binom{n}{2}\mathcal{H}^2q_0\mathcal{H}^{n-2}+\cdots+\binom{n}{n}\mathcal{H}^nq_0]. \tag{3.25}$$

Using this definition it is straightforward to verify that Eq. (3.24) is indeed the *exact operator solution* to Eq. (3.22) satisfying the initial conditions in Eq. (3.16).

Our objective is now to simplify the formal solution in Eq. (3.24) and to reexpress it in closed form. Since sines and cosines are linear combinations of exponential functions, we consider first the general problem of simplifying the Weyl-ordered product

$$\mathcal{W}(q_0e^{\mathcal{H}\tau})=\mathcal{W}\left[q_0\left(1+\mathcal{H}\tau+\frac{1}{2!}(\mathcal{H}\tau)^2+\frac{1}{3!}(\mathcal{H}\tau)^3+\cdots\right)\right]. \tag{3.26}$$

For each power of τ we reorder the operators by commuting q_0 symmetrically to the left and to the right to maintain the Hermitian form

$$\mathcal{W}(q_0)=q_0=\frac{1}{2}(q_0+q_0),$$

$$\mathcal{W}(q_0\mathcal{H})=\frac{1}{2}(q_0\mathcal{H}+\mathcal{H}q_0)=\frac{\hbar}{2}\left(q_0\frac{\mathcal{H}}{\hbar}+\frac{\mathcal{H}}{\hbar}q_0\right),$$

$$\mathcal{W}(q_0\mathcal{H}^2)=\frac{1}{4}(q_0\mathcal{H}^2+2\mathcal{H}q_0\mathcal{H}+\mathcal{H}^2q_0)=\frac{\hbar^2}{2}\left[q_0\left(\frac{\mathcal{H}^2}{\hbar^2}-\frac{1}{4}\right)+\left(\frac{\mathcal{H}^2}{\hbar^2}-\frac{1}{4}\right)q_0\right],$$

$$\mathcal{W}(q_0\mathcal{H}^3)=\frac{1}{8}(q_0\mathcal{H}^3+3\mathcal{H}q_0\mathcal{H}^2+3\mathcal{H}^2q_0\mathcal{H}+\mathcal{H}^3q_0)=\frac{\hbar^3}{2}\left[q_0\left(\frac{\mathcal{H}^3}{\hbar^3}-\frac{3}{4}\frac{\mathcal{H}}{\hbar}\right)+\left(\frac{\mathcal{H}^3}{\hbar^3}-\frac{3}{4}\frac{\mathcal{H}}{\hbar}\right)q_0\right],$$

$$\mathcal{W}(q_0\mathcal{H}^4)=\frac{1}{16}(q_0\mathcal{H}^4+4\mathcal{H}q_0\mathcal{H}^3+6\mathcal{H}^2q_0\mathcal{H}^2+4\mathcal{H}^3q_0\mathcal{H}+\mathcal{H}^4q_0)=\frac{\hbar^4}{2}\left[q_0\left(\frac{\mathcal{H}^4}{\hbar^4}-\frac{3}{2}\frac{\mathcal{H}^2}{\hbar^2}+\frac{5}{16}\right)+\left(\frac{\mathcal{H}^4}{\hbar^4}-\frac{3}{2}\frac{\mathcal{H}^2}{\hbar^2}+\frac{5}{16}\right)q_0\right], \tag{3.27}$$

and so on. This process defines a set of polynomials in the variable $\mathcal{H}/\hbar$ [15]:

$$1,\quad\frac{\mathcal{H}}{\hbar},\frac{\mathcal{H}^2}{\hbar^2}-\frac{1}{4},\quad\frac{\mathcal{H}^3}{\hbar^3}-\frac{3}{4}\frac{\mathcal{H}}{\hbar},\quad\frac{\mathcal{H}^4}{\hbar^4}-\frac{3}{2}\frac{\mathcal{H}^2}{\hbar^2}+\frac{5}{16},\quad\frac{\mathcal{H}^5}{\hbar^5}-\frac{5}{2}\frac{\mathcal{H}^3}{\hbar^3}+\frac{25}{16}\frac{\mathcal{H}}{\hbar},\quad\frac{\mathcal{H}^6}{\hbar^6}-\frac{15}{4}\frac{\mathcal{H}^4}{\hbar^4}+\frac{75}{16}\frac{\mathcal{H}^2}{\hbar^2}-\frac{61}{64}. \tag{3.28}$$

We identify these polynomials as Euler polynomials [16] in which the argument is shifted by 1/2: $E_n(=\mathcal{H}/\hbar+\frac{1}{2})$. The generating function for these nonorthogonal polynomials is given by

$$\frac{2e^{(\mathcal{H}/\hbar+1/2)\tau}}{e^{\tau}+1}=\sum_{n=0}^{\infty}\frac{\tau^n}{n!}E_n\left(\frac{\mathcal{H}}{\hbar}+\frac{1}{2}\right)\quad(|\tau|<\pi). \tag{3.29}$$

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

$$\mathcal{W}(q_0e^{\mathcal{H}\tau})=\frac{q_0e^{\mathcal{H}\tau}+e^{\mathcal{H}\tau}q_0}{2\cosh(\tau\hbar/2)}. \tag{3.30}$$

Using Eq. (3.30) the cosines and sines of our quantum solution in Eq. (3.24) can also be written in compact form when we take combinations of complex exponentials:

$$\mathcal{W}[q_0\cos(3\mathcal{H}\tau)]=\frac{q_0\cos(3\mathcal{H}\tau)+\cos(3\mathcal{H}\tau)q_0}{2\cos(3\tau\hbar/2)},$$

$$\mathcal{W}[q_0\sin(3\mathcal{H}\tau)]=\frac{q_0\sin(3\mathcal{H}\tau)+\sin(3\mathcal{H}\tau)q_0}{2\cos(3\tau\hbar/2)}. \tag{3.31}$$

Last, we substitute this result into the zeroth-order solution in Eq. (3.13) and obtain

$$\begin{aligned}Q_0(t,\tau)&=\frac{q_0\cos(t+3\mathcal{H}\tau)+\cos(t+3\mathcal{H}\tau)q_0}{2\cos(3\tau\hbar/2)}+\frac{p_0\sin(t+3\mathcal{H}\tau)+\sin(t+3\mathcal{H}\tau)p_0}{2\cos(3\tau\hbar/2)}\\&=\frac{q_0\cos(t+3\mathcal{H}\epsilon t)+\cos(t+3\mathcal{H}\epsilon t)q_0}{2\cos(3\epsilon t\hbar/2)}+\frac{p_0\sin(t+3\mathcal{H}\epsilon t)+\sin(t+3\mathcal{H}\epsilon t)p_0}{2\cos(3\epsilon t\hbar/2)},\end{aligned} \tag{3.32}$$

where we have replaced τ by ϵt. The result in Eq. (3.32) is the objective of our multiple-scale analysis. It is the quantum operator analog of Eq. (2.21). Indeed, in the limit as $\hbar \to 0$, we recover the classical multiple-scale approximation in Eq. (2.21). [To obtain this result we impose the classical initial conditions $p_0=0$ and $q_0=1$, which from Eq. (3.2) give $\mathcal{H}=\frac{1}{2}$.]

We interpret this multiple-scale approximation to the operator q as follows: In the classical case we identify the coefficient of the time variable t as a first-order approximation to the frequency shift. However, here the coefficient of t in Eq. (3.32) is an *operator*. Thus, we have derived an operator form of mass renormalization.

To understand this operator mass renormalization we must take the expectation value of Eq. (3.32) between states. Then by examining the time dependence of this matrix element we can read off 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 commutation relation (3.7). 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 $\mathcal{H}$:

$$\mathcal{H}|n\rangle=\left(n+\frac{1}{2}\right)\hbar|n\rangle. \tag{3.33}$$

Let us take the expectation value of Eq. (3.32) between the states $\langle n-1|$ and $|n\rangle$. Allowing the operator $\mathcal{H}$ to act to the left and the right using Eq. (3.33), we obtain

$$\begin{aligned}\langle n-1|Q_0|n\rangle=&\langle n-1|q_0|n\rangle\frac{\cos[t+3(n+\frac{1}{2})\hbar\epsilon t]+\cos[t+3(n-\frac{1}{2})\hbar\epsilon t]}{2\cos(3\epsilon t\hbar/2)}\\&+\langle n-1|p_0|n\rangle\frac{\sin[t+3(n+\frac{1}{2})\hbar\epsilon t]+\sin[t+3(n-\frac{1}{2})\hbar\epsilon t]}{2\cos(3\epsilon t\hbar/2)}\\=&\langle n-1|q_0|n\rangle\cos[t(1+3n\hbar\epsilon)]+\langle n-1|p_0|n\rangle\sin[t(1+3n\hbar\epsilon)],\end{aligned} \tag{3.34}$$

and we can see that the energy-level differences of the quantum oscillator are $1+3n\hbar\epsilon$.

Let us verify this result. If we set $\epsilon=0$ in Eq. (3.1), we obtain the harmonic oscillator, whose coordinate-space eigenfunctions $\psi_n(x)$ and corresponding energy eigenvalues E_n are

$$\psi_n(x)=e^{-(1/4)x^2}\mathrm{He}_n(x) \quad \text{and} \quad E_n=n+\frac{1}{2}, \tag{3.35}$$

where $\mathrm{He}_n(x)$ represents the Hermite polynomial. The first-order perturbative correction to the energy eigenvalues is obtained by computing the expectation value of the perturbation term in the Hamiltonian H:

$$\begin{aligned}E_n&=n+\frac{1}{2}+\frac{\epsilon\hbar}{4}\frac{\int_{-\infty}^{\infty}dx e^{-(1/2)x^2}[\mathrm{He}_n(x)]^2x^4}{\int_{-\infty}^{\infty}dx e^{-(1/2)x^2}[\mathrm{He}_n(x)]^2}\\&=n+\frac{1}{2}+\frac{3}{4}\epsilon\hbar(2n^2+2n+1)+O(\epsilon^2).\end{aligned} \tag{3.36}$$

If we now calculate the energy difference E_n-E_{n-1} from Eq. (3.36), we obtain

$$E_n-E_{n-1}=1+3n\hbar\epsilon+O(\epsilon^2), \tag{3.37}$$

which verifies the result in Eq. (3.34).

IV. RESUMMATION OF THE CONVENTIONAL PERTURBATION SERIES FOR THE QUANTUM ANHARMONIC OSCILLATOR

Now we turn our attention from the Heisenberg equations of motion to the Schrödinger equation and examine the behavior of the wave function. The ground-state wave function $\psi(x)$ for the quantum anharmonic oscillator satisfies the Schrödinger equation

$$\left(-\frac{d^2}{dx^2}+\frac{1}{4}x^2+\frac{1}{4}\epsilon x^4-E(\epsilon)\right)\psi(x)=0 \tag{4.1}$$

and obeys the boundary conditions

$$\psi(\pm\infty)=0. \tag{4.2}$$

We can use WKB analysis to find the large-x asymptotic behavior of the wave function $\psi(x)$. A geometrical-optics approximation gives the controlling factor (the exponential component of the leading asymptotic behavior) as

$$e^{-\sqrt{\epsilon}|x|^3/6}. \tag{4.3}$$

This result is nonperturbative in the sense that WKB is valid independent of the size of the parameter ϵ. The question addressed in this section is whether it is possible to reproduce this result using perturbation theory.

The conventional approach to solving Eq. (4.1) using Rayleigh-Schrödinger perturbation theory [5,7] represents both the eigenfunction and eigenvalue as power series in ϵ:

$$\psi(x)\sim\sum_{n=0}^{\infty}\epsilon^n y_n(x)\quad\text{and}\quad E(\epsilon)\sim\sum_{n=0}^{\infty}\epsilon^n E_n. \tag{4.4}$$

Note that we use the asymptotic symbol $\sim$ because, as is well known, the conventional perturbation series for the anharmonic oscillator diverges.

Equations (4.1) and (4.2) are homogeneous, so we are free to adopt the normalization condition $\psi(0)=1$, which translates into

$$y_0(0)=1\quad\text{and}\quad y_n(0)=0\quad(n>0). \tag{4.5}$$

The unperturbed (harmonic-oscillator) solutions corresponding to $\epsilon=0$ are

$$y_0(x)=e^{-x^2/4}\quad\text{and}\quad E_0=\frac{1}{2}. \tag{4.6}$$

In Ref. [5] it is shown that for all n, $y_n(x)$ is a product of the zeroth-order approximation to the wave function $y_0(x)$ given in Eq. (4.6) multiplied by a polynomial $P_n(x)$:

$$y_n=e^{-x^2/4}P_n(x). \tag{4.7}$$

Substituting Eq. (4.7) into Eq. (4.1), we obtain the recursion formula for the polynomials:

$$P_n''(x)-xP_n'(x)=\frac{1}{4}x^4P_{n-1}(x)-\sum_{j=0}^{n-1}P_j(x)E_{n-j}. \tag{4.8}$$

The form of this recursion relation is generic. It is a typical recursive structure that arises in all perturbative calculations; to wit, the homogeneous part of this recursion relation is the same for all n while the inhomogeneous part contains all previous polynomials. It is this kind of recursive structure that is responsible for successive orders of perturbation theory being resonantly coupled. Here, the resonant coupling causes the degree of the polynomials to grow with n; $P_n(x)$ is a polynomial of degree $2n$ in the variable x^2:

$$P_0(x)=1,$$

$$P_1(x)=-\frac{3}{2}\left(\frac{x}{2}\right)^2-\left(\frac{x}{2}\right)^4,$$

$$P_2(x)=\frac{21}{4}\left(\frac{x}{2}\right)^2+\frac{31}{8}\left(\frac{x}{2}\right)^4+\frac{13}{6}\left(\frac{x}{2}\right)^6+\frac{1}{2}\left(\frac{x}{2}\right)^8,$$

$$P_3(x)=-\frac{333}{8}\left(\frac{x}{2}\right)^2-\frac{243}{8}\left(\frac{x}{2}\right)^4-\frac{271}{16}\left(\frac{x}{2}\right)^6-\frac{47}{8}\left(\frac{x}{2}\right)^8-\frac{17}{12}\left(\frac{x}{2}\right)^{10}-\frac{1}{6}\left(\frac{x}{2}\right)^{12},$$

$$P_4(x)=\frac{30\,885}{64}\left(\frac{x}{2}\right)^2+\frac{2777}{8}\left(\frac{x}{2}\right)^4+\frac{18\,461}{96}\left(\frac{x}{2}\right)^6+\frac{9195}{128}\left(\frac{x}{2}\right)^8+\frac{979}{48}\left(\frac{x}{2}\right)^{10}+\frac{599}{144}\left(\frac{x}{2}\right)^{12}+\frac{7}{12}\left(\frac{x}{2}\right)^{14}+\frac{1}{24}\left(\frac{x}{2}\right)^{16},$$

$$P_5(x)=-\frac{916\,731}{128}\left(\frac{x}{2}\right)^2-\frac{651\,363}{128}\left(\frac{x}{2}\right)^4-\frac{89\,673}{32}\left(\frac{x}{2}\right)^6-\frac{69\,107}{64}\left(\frac{x}{2}\right)^8-\frac{250\,183}{768}\left(\frac{x}{2}\right)^{10}-\frac{29\,177}{384}\left(\frac{x}{2}\right)^{12}-\frac{1325}{96}\left(\frac{x}{2}\right)^{14}$$
$$-\frac{269}{144}\left(\frac{x}{2}\right)^{16}-\frac{25}{144}\left(\frac{x}{2}\right)^{18}-\frac{1}{120}\left(\frac{x}{2}\right)^{20},$$

$$P_6(x)=\frac{65\,518\,401}{512}\left(\frac{x}{2}\right)^2+\frac{23\,046\,319}{256}\left(\frac{x}{2}\right)^4+\frac{75\,770\,813}{1536}\left(\frac{x}{2}\right)^6+\frac{2\,476\,011}{128}\left(\frac{x}{2}\right)^8+\frac{9\,259\,481}{1536}\left(\frac{x}{2}\right)^{10}+\frac{13\,796\,435}{9216}\left(\frac{x}{2}\right)^{12}$$
$$+\frac{77\,173}{256}\left(\frac{x}{2}\right)^{14}+\frac{112\,483}{2304}\left(\frac{x}{2}\right)^{16}+\frac{4055}{648}\left(\frac{x}{2}\right)^{18}+\frac{349}{576}\left(\frac{x}{2}\right)^{20}+\frac{29}{720}\left(\frac{x}{2}\right)^{22}+\frac{1}{720}\left(\frac{x}{2}\right)^{24}. \tag{4.9}$$

For $n>0$ the general form of the polynomial is

$$P_n(x)=\sum_{k=1}^{2n} C_{n,k}\left(-\frac{1}{2}x^2\right)^k. \tag{4.10}$$

Note that by virtue of Eq. (4.5) the polynomials $P_n(x)$ have *no* constant term when $n>0$.

We can derive a formula for E_n and a recursion relation for the coefficients $C_{n,k}$ by substituting Eq. (4.10) into Eq. (4.8) to obtain, for $n>0$,

$$C_{n,1}=E_n,$$
$$2kC_{n,k}+C_{n-1,k-2}=-(k+1)(2k+1)C_{n,k+1}+\sum_{j=1}^{n-1} C_{j,k}C_{n-j,1}. \tag{4.11}$$

The coefficients $C_{n,k}$ form a triangular array in the sense that the degree of the polynomials increases with n. The convolution in Eq. (4.11) makes this recursion relation highly nontrivial. However, for all n it is possible to find $C_{n,2n}$, the coefficient of the *highest power* of x. This is an exact analog of finding the coefficient of the highest power of t (most secular term) in nth order in perturbation theory for the classical anharmonic oscillator. By setting $k=2n$ in Eq. (4.11), we see that $C_{n,2n}$ satisfies the simple linear recursion relation

$$4nC_{n,2n}+C_{n-1,2n-2}=0, \tag{4.12}$$

whose solution is

$$C_{n,2n}=\left(-\frac{1}{4}\right)^n\frac{1}{n!}. \tag{4.13}$$

To study the behavior of the wave function $\psi(x)$ for large x, we approximate $\psi(x)$ by resumming the perturbation series in Eq. (4.4) and keeping just the *highest power* of x in every order. Using Eq. (4.13) we obtain a simple exponential approximation to $\psi(x)$:

$$\sum_{n=0}^{\infty}\epsilon^n e^{-x^2/4}\frac{(-1)^n}{n!16^n}x^{4n}=e^{-x^2/4}e^{-\epsilon x^4/16}. \tag{4.14}$$

For the classical anharmonic oscillator this approach also gives an exponential approximation [see Eq. (2.11)]. However, the classical and quantum anharmonic oscillators are evidently quite different; although we have summed the most secular terms to all orders in perturbation theory, the result in Eq. (4.14) is *not* the correct behavior of the wave function $\psi(x)$ for large x because it decays to zero too rapidly. The correct behavior from WKB theory is an exponential of a cubic [see Eq. (4.3)] and not an exponential of a quartic.

Can we improve our estimate of $\psi(x)$ by including $C_{n,2n-1}$, the coefficient of the *next highest power* of x, in our summation? This coefficient satisfies the inhomogeneous difference equation obtained by setting $k=2n-1$ in Eq. (4.11):

$$(4n-2)C_{n,2n-1}+C_{n-1,2n-3}=-2n(4n-1)C_{n,2n}=-2n(4n-1)\left(-\frac{1}{4}\right)^n\frac{1}{n!}. \tag{4.15}$$

The solution to this inhomogeneous equation is

$$C_{n,2n-1}=-\left(-\frac{1}{4}\right)^n\frac{1}{n!}\frac{n}{3}(4n+5). \tag{4.16}$$

If we include this formula in the resummation to all orders, we obtain the result in Eq. (4.14) now multiplied by a polynomial:

$$e^{-x^2/4}e^{-\epsilon x^4/16}\left(1-\frac{3}{8}\epsilon x^2+\frac{1}{96}\epsilon^2x^6\right). \tag{4.17}$$

We have again failed to obtain the correct large-x behavior of $\psi(x)$. Nevertheless, let us continue to reorganize the perturbation series. Setting $k=2n-2$ in Eq. (4.11), we get

$$(4n-4)C_{n,2n-2}+C_{n-1,2n-4}=-(2n-1)(4n-3)C_{n,2n-1}+\frac{3}{4}C_{n-1,2n-2}, \tag{4.18}$$

whose solution is

$$C_{n,2n-2}=\left(-\frac{1}{4}\right)^n\frac{1}{n!}\frac{n(n-1)}{18}(16n^2+64n+87). \tag{4.19}$$

The next few coefficients are

$$C_{n,2n-3}=-\left(-\frac{1}{4}\right)^n\frac{1}{n!}\frac{n(n-1)}{162}(64n^4+400n^3+764n^2-433n+390), \tag{4.20}$$

$$C_{n,2n-4}=\left(-\frac{1}{4}\right)^n\frac{1}{n!}\frac{n(n-1)(n-2)}{1944}(256n^5+2816n^4+11\,744n^3+18\,304n^2+34\,209n+70\,029),$$

$$C_{n,2n-5}=-\left(-\frac{1}{4}\right)^n\frac{1}{n!}\frac{n(n-1)(n-2)}{29\,160}(1024n^7+14\,592n^6+74\,368n^5+106\,080n^4+45\,316n^3$$
$$+143\,073n^2-2\,392\,803n+3\,967\,380),$$

$$C_{n,2n-6}=\left(-\frac{1}{4}\right)^n\frac{1}{n!}\frac{n(n-1)(n-2)(n-3)}{524\,880}(4096n^8+86\,016n^7+718\,080n^6$$
$$+2\,799\,360n^5+6\,702\,384n^4+16\,486\,704n^3$$
$$+16\,745\,975n^2+180\,087\,585n+415\,966\,860).$$

Evidently, the coefficient $C_{n,2n-j}$ has the general form of a polynomial in n of degree $2j$ multiplied by $(-4)^{-n}/n!$.

When we sum these coefficients to all orders, we obtain a totally new sequence of polynomials (displayed below in square brackets) in the variable ϵx^4:

$$e^{-x^2/4}e^{-\epsilon x^4/16}\left\{1+\left[-\frac{3}{2}\epsilon\left(\frac{x}{2}\right)^2+\frac{2}{3}\epsilon^2\left(\frac{x}{2}\right)^6\right]+\left[\frac{31}{8}\epsilon^2\left(\frac{x}{2}\right)^4-2\epsilon^3\left(\frac{x}{2}\right)^8+\frac{2}{9}\epsilon^4\left(\frac{x}{2}\right)^{12}\right]\right.$$
$$+\left[\frac{21}{4}\epsilon^2\left(\frac{x}{2}\right)^2-\frac{187}{16}\epsilon^3\left(\frac{x}{2}\right)^6+\frac{73}{12}\epsilon^4\left(\frac{x}{2}\right)^{10}-\epsilon^5\left(\frac{x}{2}\right)^{14}+\frac{4}{81}\epsilon^6\left(\frac{x}{2}\right)^{18}\right]+\left[-\frac{243}{8}\epsilon^3\left(\frac{x}{2}\right)^4+\frac{5307}{128}\epsilon^4\left(\frac{x}{2}\right)^8-\frac{58}{3}\epsilon^5\left(\frac{x}{2}\right)^{12}\right.$$
$$+\frac{133}{36}\epsilon^6\left(\frac{x}{2}\right)^{16}-\frac{8}{27}\epsilon^7\left(\frac{x}{2}\right)^{20}+\frac{2}{243}\epsilon^8\left(\frac{x}{2}\right)^{24}\left.\right]+\left[-\frac{333}{8}\epsilon^3\left(\frac{x}{2}\right)^2+\frac{14\,465}{96}\epsilon^4\left(\frac{x}{2}\right)^6-\frac{39\,493}{256}\epsilon^5\left(\frac{x}{2}\right)^{10}+\frac{12\,463}{192}\epsilon^6\left(\frac{x}{2}\right)^{14}\right.$$
$$-\frac{313}{24}\epsilon^7\left(\frac{x}{2}\right)^{18}+\frac{211}{162}\epsilon^8\left(\frac{x}{2}\right)^{22}-\frac{5}{81}\epsilon^9\left(\frac{x}{2}\right)^{26}+\frac{4}{3645}\epsilon^{10}\left(\frac{x}{2}\right)^{30}\left.\right]$$
$$+\left[\frac{2777}{8}\epsilon^4\left(\frac{x}{2}\right)^4-\frac{46\,891}{64}\epsilon^5\left(\frac{x}{2}\right)^8+\frac{5\,444\,579}{9216}\epsilon^6\left(\frac{x}{2}\right)^{12}-\frac{14\,497}{64}\epsilon^7\left(\frac{x}{2}\right)^{16}+\frac{79\,357}{1728}\epsilon^8\left(\frac{x}{2}\right)^{20}-\frac{833}{162}\epsilon^9\left(\frac{x}{2}\right)^{24}\right.$$
$$\left.+\frac{307}{972}\epsilon^{10}\left(\frac{x}{2}\right)^{28}-\frac{4}{405}\epsilon^{11}\left(\frac{x}{2}\right)^{32}+\frac{4}{32\,805}\epsilon^{12}\left(\frac{x}{2}\right)^{36}\right]+\cdots\left.\right\}. \tag{4.21}$$

The original form of the perturbation series in Eqs. (4.4) and (4.7) has undergone a remarkable transmutation. The original polynomials $P_n(x)$ have been absorbed and the wave function $\psi(x)$ is now represented as a more elaborate exponential multiplying a new class of polynomials. [We can, of course, generate these polynomials directly from the Schrödinger equation (4.1) using a recursion relation similar to that in Eq. (4.8).]

Let us perform a further resummation procedure. That is, for this new set of polynomials we determine the coefficient of the highest power of x,

$$\left(\frac{2}{3}\right)^n\left(\frac{x}{2}\right)^{6n}\frac{1}{n!}\epsilon^{2n}, \tag{4.22}$$

the coefficient of the second-highest power of x,

$$-\frac{9}{4}\left(\frac{2}{3}\right)^n\left(\frac{x}{2}\right)^{6n-4}\frac{1}{n!}\epsilon^{2n-1}n^2, \tag{4.23}$$

the coefficient of the third-highest power of x,

$$\frac{9}{32}\left(\frac{2}{3}\right)^n\left(\frac{x}{2}\right)^{6n-8}\frac{1}{n!}\epsilon^{2n-2}n(n-1)(9n^2-3n+1), \tag{4.24}$$

the coefficient of the fourth-highest power of x,

$$-\frac{27}{128}\left(\frac{2}{3}\right)^n\left(\frac{x}{2}\right)^{6n-12}\frac{1}{n!}\epsilon^{2n-3}n(n-1)(n-2)(9n^3-9n^2+7n+4), \tag{4.25}$$

and so on.

Having discovered these formulas we can now sum over n. This further reorganization of the perturbation series gives a *new* approximation to $\psi(x)$ as an exponential multiplied by yet another set of polynomials, this time in the variable ϵ^2x^6:

$$e^{-x^2/4}e^{-\epsilon x^4/16}e^{\epsilon^2 x^6/96}\left\{1-\left[\frac{3}{2}\epsilon\left(\frac{x}{2}\right)^2+\epsilon^3\left(\frac{x}{2}\right)^8\right]+\left[\frac{31}{8}\epsilon^2\left(\frac{x}{2}\right)^4+\frac{7}{2}\epsilon^4\left(\frac{x}{2}\right)^{10}+\frac{1}{2}\epsilon^6\left(\frac{x}{2}\right)^{16}\right]\right.$$
$$\left.-\left[\frac{187}{16}\epsilon^3\left(\frac{x}{2}\right)^6+\frac{277}{24}\epsilon^5\left(\frac{x}{2}\right)^{12}+\frac{11}{4}\epsilon^7\left(\frac{x}{2}\right)^{18}+\frac{1}{6}\epsilon^9\left(\frac{x}{2}\right)^{24}\right]+\cdots\right\}. \tag{4.26}$$

For these new polynomials the term containing the highest power of x has the form

$$(-1)^n\left(\frac{x}{2}\right)^{8n}\frac{1}{n!}\epsilon^{3n}, \tag{4.27}$$

and the term containing the second-highest power of x has the form

$$\frac{1}{2}(-1)^n\left(\frac{x}{2}\right)^{8n-6}\frac{1}{n!}\epsilon^{3n-2}n(4n-1). \tag{4.28}$$

Again, we reorganize the perturbation series by summing over all n. This resummation gives yet another representation for $\psi(x)$ as an exponential multiplied by a new set of polynomials, this time in the variable ϵ^3x^8:

$$e^{-x^2/4}e^{-\epsilon x^4/16}e^{\epsilon^2 x^6/96}e^{-\epsilon^3 x^8/256}\left\{1+\left[-\frac{3}{2}\epsilon\left(\frac{x}{2}\right)^2+2\epsilon^4\left(\frac{x}{2}\right)^{10}\right]+\cdots\right\}. \tag{4.29}$$

For these polynomials we identify the term containing the highest power of x,

$$2^n\left(\frac{x}{2}\right)^{10n}\frac{1}{n!}\epsilon^{4n}, \tag{4.30}$$

and we reorganize the perturbation series again by summing over all n. This resummation gives a new exponential and a new set of polynomials, this time in the variable ϵ^4x^{10}:

$$e^{-x^2/4}e^{-\epsilon x^4/16}e^{\epsilon^2 x^6/96}e^{-\epsilon^3 x^8/256}e^{\epsilon^4 x^{10}/512}\{1+\cdots\}. \tag{4.31}$$

We can continue this process indefinitely. With each iterative reorganization of the perturbation series we generate a new exponential multiplied by new polynomials. However, we have not attained our original goal of deriving the exponential behavior in Eq. (4.3) from the weak-coupling perturbation series in powers of ϵ. Indeed, it seems impossible for our approach to succeed because at each stage in the reorganization of the perturbation series the variable x appears only in *even* powers. How can we ever obtain the exponential of a *cubic*?

There is a simple and direct answer to this question. We merely recognize that the exponent in Eq. (4.31) is the beginning of a binomial series:

$$-\frac{x^2}{4}-\frac{1}{16}\epsilon x^4+\frac{1}{96}\epsilon^2x^6-\frac{1}{256}\epsilon^3x^8+\frac{1}{512}\epsilon^4x^{10}+\cdots$$
$$=\frac{1}{6\epsilon}[1-(1+\epsilon x^2)^{3/2}]. \tag{4.32}$$

If we now let x be large ($\epsilon x^2\gg 1$), we recover the asymptotic behavior in Eq. (4.3):

$$\exp\left\{\frac{1}{6\epsilon}[1-(1+\epsilon x^2)^{3/2}]\right\}\sim e^{-\sqrt{\epsilon}|x|^3/6}\quad(|x|\to\infty). \tag{4.33}$$

Let us examine more deeply what happens at each reorganization of the perturbation series. At the first resummation we sum over terms of the form $\epsilon^n x^{4n}$ and treat ϵx^4 as small. Thus, while x may be large compared with 1, it cannot be too large; x must satisfy the asymptotic bound $x\ll\epsilon^{-1/4}$. At the next reorganization we sum over terms of the form $\epsilon^{2n}x^{6n}$ and treat ϵ^2x^6 as small. This resummation is valid in the larger region $x\ll\epsilon^{-1/3}$. At the next level we sum over terms of the form $\epsilon^{3n}x^{8n}$ and treat ϵ^3x^8 as small. Hence, this resummation is valid in a still larger region, $x\ll\epsilon^{-3/8}$. At the jth iteration the range of x increases to $x\ll\epsilon^{j}/(2j+2)$. Clearly, as $j\to\infty$, we obtain an estimate of the wave function $\psi(x)$ that is valid for x as large as $\epsilon^{-1/2}$. It is only when x is this large that the ϵx^4 term in the Schrödinger equation (4.1) becomes comparable in size to the x^2 term. Thus, after a finite number of reorderings of the perturbation series, we cannot expect to reproduce exactly the exponential behavior in Eq. (4.3).

Nevertheless, at each stage of the resummation process we observe precursors of the exponential behavior in Eq. (4.3). To demonstrate this, we examine the structure of the exponent in Eq. (4.31), in which we factor out the first term:

$$-\frac{x^2}{4}\left(1+\frac{1}{4}\epsilon x^2-\frac{1}{24}\epsilon^2x^4+\frac{1}{64}\epsilon^3x^6-\frac{1}{128}\epsilon^4x^8+\cdots\right). \tag{4.34}$$

At the first iteration, which is valid for $x\ll\epsilon^{-1/4}$, we neglect all terms in Eq. (4.34) beyond $\frac{1}{4}\epsilon x^2$ (because they are small compared with 1) and replace this series by

$$-\frac{x^2}{4}\left(1+\frac{1}{2}\epsilon x^2\right)^{1/2}. \tag{4.35}$$

At the second iteration, which is valid for $x \ll \epsilon^{-1/3}$, we neglect all terms in Eq. (4.34) beyond $-1/24\epsilon^2x^4$ and replace the series by

$$-\frac{x^2}{4}\left(1+\epsilon x^2+\frac{5}{24}\epsilon^2x^4\right)^{1/4}. \tag{4.36}$$

At the next two iterations we have

$$-\frac{x^2}{4}\left(1+\frac{3}{2}\epsilon x^2+\frac{11}{16}\epsilon^2x^4+\frac{3}{32}\epsilon^3x^6\right)^{1/6} \tag{4.37}$$

and

$$-\frac{x^2}{4}\left(1+2\epsilon x^2+\frac{17}{12}\epsilon^2x^4+\frac{5}{12}\epsilon^3x^6+\frac{47}{1152}\epsilon^4x^8\right)^{1/8}. \tag{4.38}$$

Now, let x be large. In each of the above formulas we obtain a cubic in x. Moreover, this cubic is multiplied by $-\sqrt{\epsilon}$ and the numerical coefficients of the cubic approach $\frac{1}{6}$:

$$\frac{1}{4\sqrt{2}}=\frac{1}{5.656\,85},$$

$$\frac{1}{4(24/5)^{1/4}}=\frac{1}{5.920\,66},$$

$$\frac{1}{4(32/3)^{1/6}}=\frac{1}{5.934\,69},$$

$$\frac{1}{4(1152/47)^{1/8}}=\frac{1}{5.966\,63}. \tag{4.39}$$

It is now clear how it is possible to obtain a cubic in x from only even powers of x.

Having given a detailed discussion of the exponential prefactor that emerges at each stage of the resummation process, we conclude this section by describing the structures of the polynomials that arise at every stage. Let N represent the number of resummations that we have performed. Then for each value of N we can express the wave function $\psi(x)$ as an exponential multiplied by a sum over polynomials. We have established that after N resummations the exponential factor has the form

$$\exp\left[-\frac{x^2}{4}\sum_{n=0}^{N}\frac{\Gamma(3/2)}{\Gamma(3/2-n)(n+1)!}(\epsilon x^2)^n\right]. \tag{4.40}$$

At each stage N in the resummation process the argument of the polynomials changes so we denote the argument by z_N, where

$$z_N \equiv \epsilon^N\left(\frac{x^2}{4}\right)^{N+1}. \tag{4.41}$$

In general, the wave function is a product of the exponential factor multiplied by a power series in the variable

$$y \equiv \frac{1}{4}\epsilon x^2. \tag{4.42}$$

We represent the coefficient of y^n at the Nth resummation by the notation $\mathcal{P}_n^{(N)}(z_N)$. Thus,

$$\psi(x)=\exp\left[-\frac{x^2}{4}\sum_{n=0}^{N}\frac{\Gamma(\frac{3}{2})}{\Gamma(\frac{3}{2}-n)(n+1)!}(\epsilon x^2)^n\right]\sum_{n=0}^{\infty}y^n\mathcal{P}_n^{(N)}(z_N). \tag{4.43}$$

We now describe the structure of $\mathcal{P}_n^{(N)}(z_N)$. For sufficiently large N, $N>n-2$, $\mathcal{P}_n^{(N)}$ is a polynomial of degree n. However, when $N \leqslant n-2$, negative powers are present. The largest negative power of z_N is $z_N^{-(n-N-1)}$. Thus, in the range from $N=0$ to $N=n-2$, $\mathcal{P}_n^{(N)}(z_N)$ contains all powers of z_N from $z_N^{-(n-N-1)}$ to z_N^n. But when $N>n-2$, $\mathcal{P}_n^{(N)}(z_N)$ contains all powers of z_N from z_N^0 to z_N^n.

We now give some formulas for the functions $\mathcal{P}_n^{(N)}$. For all N, $\mathcal{P}_0^{(N)}$ is extremely simple:

$$\mathcal{P}_0^{(N)}(z_N)=1. \tag{4.44}$$

We have found a closed-form general expression for $\mathcal{P}_1^{(N)}$ valid for all N:

$$\mathcal{P}_1^{(N)}(z_N)=-\frac{3}{2}-2(-1)^N\frac{(2N)!}{N!(N+2)!}z_N. \tag{4.45}$$

The closed-form expression for $\mathcal{P}_2^{(N)}$ is more complicated:

$$\mathcal{P}_2^{(N)}(z_N)=\begin{cases}\dfrac{21}{4}z_0^{-1}+\dfrac{31}{8}+\dfrac{13}{6}z_0+\dfrac{1}{2}z_0^2 & (N=0),\\[2ex] \dfrac{31}{8}-(-1)^N\dfrac{(11N+13)(2N)!}{N!(N+3)!}z_N+2\left[\dfrac{(2N)!}{N!(N+2)!}\right]^2z_N^2 & (N>0).\end{cases} \tag{4.46}$$

The expression for $\mathcal{P}_3^{(N)}$ is still more complicated:

$$\mathcal{P}_3^{(N)}(z_N)=\begin{cases} -\frac{333}{8}z_0^{-2}-\frac{243}{8}z_0^{-1}-\frac{271}{16}-\frac{47}{8}z_0-\frac{17}{12}z_0^2-\frac{1}{6}z_0^3 \quad (N=0), \\ \frac{21}{4}z_1^{-1}-\frac{187}{16}+\frac{73}{12}z_1-z_1^2+\frac{4}{81}z_1^3 \quad (N=1), \\ -\frac{187}{16}+b_N z_N+c_N z_N^2-(-1)^N\frac{4}{3}\left[\frac{(2N)!}{N!(N+2)!}\right]^3 z_N^3 \quad (N>1), \end{cases} \tag{4.47}$$

where b_N and c_N are rational numbers.

Ginsburg and Montroll [17] attempted to approximate the wave function for the anharmonic oscillator by a sequence of exponentials of fractional powers of polynomials. In this respect their work is superficially similar to ours. However, they did not generate these polynomials from the Rayleigh-Schrödinger perturbation series; rather, they attempted to *fit* the small-ϵ and large-x behaviors of $\psi(x)$ and then to deduce formulas for the eigenvalues. Their work represented the wave function $\psi(x)$ by an exponential function only, whereas in our work there are always polynomials $\mathcal{P}$ multiplying the exponential structure. These polynomials will never disappear, even after an infinite number of resummations, because they express the *physical-optics* correction to the geometrical-optics approximation to the wave function. The exponential in Eq. (4.3) is only the geometrical-optics approximation.

V. MULTIPLE-SCALE PERTURBATION THEORY APPLIED TO THE SCHRÖDINGER EQUATION FOR THE ANHARMONIC OSCILLATOR

In this section we attempt to obtain the large-x asymptotic behavior of the wave function $\psi(x)$ by applying MSPT directly to the Schrödinger equation (4.1). We will see that multiple-scale analysis gives the results of the previous section but it avoids the need to resum the perturbation series.

Recall that in Sec. IV we showed that the asymptotic form of the wave function as the exponential of a cubic could only be obtained after an infinite number of resummations. Since multiple-scale analysis is equivalent to resumming the most secular terms in the perturbation series, we expect that at every order of MSPT we will find a result similar in structure to the forms of the previous section. Thus, we expect that leading-order MSPT based on just two scales will fail to generate the correct cubic asymptotic behavior of the wave-function in Eq. (4.3). However, we expect that as we include more and more scales in the MSPT we will obtain a series like that in Eqs. (4.32) and (4.33).

We will see that the application of MSPT to the Schrödinger equation (2.1) is not straightforward. MSPT is conventionally applied to systems that reduce to classical harmonic oscillators when the perturbation parameter vanishes so that long scales are equal to the short scale multiplied by increasing powers of the perturbation parameter ϵ. The multiple-scale analysis that we perform here is unusual because, as we have already see in Sec. IV, the long scales are now proportional to increasing powers of x^2 as well as ϵ. In the following generalization of MSPT we will show how the definition of the long scales relative to the short scale x can be deduced from the formalism and that secularity has a natural analogue in the behavior of the wave function for large x.

To illustrate our procedure we begin by performing a multiple-scale analysis involving only two scales. (A higher-order analysis will be given later on.) We assume a perturbative solution to Eq. (4.1) of the form

$$\psi(x)=G_0(x,\xi_1)+\epsilon G_1(x,\xi_1)+O(\epsilon^2), \tag{5.1}$$

where the short scale is x and the long scale ξ_1 is an *unknown* function of x: $\xi_1=\epsilon f_1(x)$. (We use the subscript 1 to indicate that this is the *first* of a hierarchy of longer and longer scales.) This assumption is reminiscent of the method of stretched coordinates [3].

Using the chain rule we calculate the first two derivatives of $\psi(x)$:

$$\frac{d\psi}{dx}=\frac{\partial G_0}{\partial x}+\epsilon\left(\frac{\partial G_0}{\partial \xi_1}\frac{df_1}{dx}+\frac{\partial G_1}{\partial x}\right)+O(\epsilon^2),$$

$$\frac{d^2\psi}{dx^2}=\frac{\partial^2 G_0}{\partial x^2}+\epsilon\left(\frac{\partial^2 G_0}{\partial \xi_1 \partial x}\frac{df_1}{dx}+\frac{\partial G_0}{\partial \xi_1}\frac{d^2 f_1}{dx^2}+\frac{\partial^2 G_1}{\partial x^2}\right)+O(\epsilon^2). \tag{5.2}$$

Next, we substitute Eqs. (5.1) and (5.2) into the Schrödinger equation and collect coefficients of powers of ϵ. To order ϵ^0 we obtain the Schrödinger equation for the quantum harmonic oscillator:

$$-\frac{\partial^2 G_0}{\partial x^2}+\left(\frac{1}{4}x^2-\frac{1}{2}\right)G_0=0. \tag{5.3}$$

The solution to this equation that is normalizable is

$$G_0(x,\xi_1)=A(\xi_1)e^{-(1/4)x^2}, \tag{5.4}$$

where $A(\xi_1)$ is an unknown function of the long scale ξ_1.

To order ϵ^1 we obtain

$$-\frac{\partial^2 G_1}{\partial x^2}+\left(\frac{1}{4}x^2-\frac{1}{2}\right)G_1=2\frac{\partial^2 G_0}{\partial \xi_1 \partial x}\frac{df_1}{dx}+\frac{\partial G_0}{\partial \xi_1}\frac{d^2 f_1}{dx^2}-\frac{1}{4}x^4 G_0+E_1 G_0, \tag{5.5}$$

where E_1 is the first-order correction to the energy eigenvalue.

Substituting the solution for G_0 into Eq. (5.5) gives

$$-\frac{\partial^2 G_1}{\partial x^2}+\left(\frac{1}{4}x^2-\frac{1}{2}\right)G_1 = e^{-(1/4)x^2}\left[-\frac{dA}{d\xi_1}\left(x\frac{df_1}{dx}-\frac{d^2f_1}{dx^2}\right)-A\left(\frac{1}{4}x^4-E_1\right)\right]. \tag{5.6}$$

We now make the crucial argument in this procedure. By analogy with conventional MSPT we do not want G_1 to satisfy an inhomogeneous equation driven by its homogeneous solution G_0 because this will give a contribution to G_1 that may decay less quickly than G_0 for large x. For example, if the square bracket in Eq. (5.6) were a constant, then G_1 would grow like $G_0 \ln x$ for large x. We thus require that the square bracket on the right side of Eq. (5.6) vanish identically. Of course, one cannot give a logical argument that this expression must vanish. Rather, we exploit the functional degree of freedom that we introduced in Eq. (5.1) when we replaced a function of one variable by a function of two variables and simply *demand that the square bracket vanish identically*.

We proceed as one does when performing a separation of variables for a partial differential equation. The vanishing of the expression in square brackets gives *two* ordinary differential equations, one for f_1 and one for A. Apart from constants of integration that are irrelevant because they scale out, we obtain

$$f_1(x)=\frac{1}{16}x^4+\frac{3}{8}x^2 \quad \text{and} \quad E_1=\frac{3}{4}, \tag{5.7}$$

which fully defines the scale $\xi_1=\epsilon(\frac{1}{16}x^4+\frac{3}{8}x^2)$. Note that E_1 computed here is the usual perturbative correction to the eigenvalue determined from Eq. (4.8). Also, we have

$$A(\xi_1)=e^{-\xi_1}. \tag{5.8}$$

Finally, we use the expression for ξ_1 in terms of x to rewrite the solution for G_0:

$$G_0=e^{-(1/4)x^2[1+(3/2)\epsilon]-(1/16)\epsilon x^4}. \tag{5.9}$$

Observe that this generalized multiple-scale procedure leads to a solution that incorporates not only the next term in the expansion of the exponent [see Eq. (4.32)] but also contains a correction to the $\frac{1}{4}x^2$ term. If we expand the exponent, we see that this correction gives the *constant term* in the polynomial $\mathcal{P}_1^{(N)}(z_N)$ in Eq. (4.45).

We now perform the multiple-scale approximation to higher order. We will see that our multiple-scale procedure determines the new long-scale variables required to describe the behavior of the wave function for large x. Moreover, the higher-order calculation predicts exactly the higher-order corrections to the energy eigenvalue. We generalize the first-order calculation by introducing more long-scale variables $\xi_2=\epsilon^2 f_2(x)$, $\xi_3=\epsilon^3 f_3(x)$, and so on. The functions f_n are determined from the requirement that the right side of the differential equation for G_n vanish. This requirement yields the new dependence of G_0 on ξ_n.

To order ϵ^2 this procedure yields

$$\xi_2=\epsilon^2\left(\frac{1}{96}x^6+\frac{11}{64}x^4+\frac{21}{8}x^2\right) \quad \text{and} \quad E_2=-\frac{21}{8}, \tag{5.10}$$

and

$$G_0(x)=\exp\left[\frac{1}{4}x^2\left(1+\frac{3}{2}\epsilon-\frac{21}{4}\epsilon^2\right)-\frac{1}{16}\epsilon x^4\left(1-\frac{11}{4}\epsilon\right)+\frac{1}{96}\epsilon^2 x^6\right]. \tag{5.11}$$

To order ϵ^3 we have

$$\xi_3=\epsilon^3\left(\frac{1}{256}x^8+\frac{21}{192}x^6+\frac{45}{32}x^4+\frac{333}{32}x^2\right)$$

and

$$E_3=\frac{333}{16}, \tag{5.12}$$

and

$$G_0(x)=\exp\left[-\frac{1}{4}x^2\left(1+\frac{3}{2}\epsilon-\frac{21}{4}\epsilon^2+\frac{333}{8}\epsilon^3\right)-\frac{1}{16}\epsilon x^4\left(1-\frac{11}{4}\epsilon+\frac{45}{2}\epsilon^2\right)+\frac{1}{96}\epsilon^2 x^6\left(1-\frac{21}{2}\epsilon\right)-\frac{1}{256}\epsilon^3 x^8\right]. \tag{5.13}$$

Observe the pattern that develops. Every new order in MSPT reproduces a new term in the expansion of the exponent in Eq. (4.32) together with x-dependent corrections to the wave function in the exponential. To recover the sequence polynomials $\mathcal{P}_1$, $\mathcal{P}_2$, $\mathcal{P}_3$, ..., which are discussed in Sec. IV one need only expand the exponentials.

ACKNOWLEDGMENTS

We thank T. T. Wu for a very helpful discussion. One of us, C.M.B., thanks the Fulbright Foundation, the PPARC, and the U.S. Department of Energy for financial support. One of us, L.M.A.B., thanks JNICT-*Programa Praxis XXI* for financial support under Contract No. BD 2243/92. This work was supported in part by the European Commission under the Human Capital and Mobility Programme, Contract No. CHRX-CT94-0423.

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