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Perturbation theory and the classical limit of quantum mechanics

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We consider the classical limit of quantum mechanics from the viewpoint of perturbation theory. The main focus is time dependent perturbation theory, in particular, the time evolution of a harmonic oscillator coherent state in an anharmonic potential. We explore in detail a perturbation method introduced by Bhaumik and Dutta-Roy [J. Math. Phys. **16**, 1131 (1975)] and resolve several complications that arise when this method is extended to second order. A classical limit for coherent states used by the above authors is then applied to the quantum perturbation expansions and, to second order, the classical Poincaré–Lindstedt series is retrieved. We conclude with an investigation of the connection between the classical limits of time dependent and time independent perturbation theories, respectively. © 1997 American Institute of Physics. [S0022-2488(97)01406-0]

I. INTRODUCTION

This paper represents a continuation of a series of investigations of classical limits of quantum mechanical perturbation expansions. Previously¹ we showed that the classical mechanical (CM) version of the Hellmann–Feynman (HF) theorem could be used to generate the CM Poincaré–von Zeipel perturbation expansions² of a periodic orbit with fixed classical action J . The CM Poincaré–von Zeipel perturbation expansion associated with a periodic orbit having action J can be obtained from the quantum mechanical (QM) Rayleigh–Schrödinger expansion of an eigenstate by the following classical limit: $n \rightarrow \infty, \hbar \rightarrow 0$, with $n\hbar = J$. This limit was first applied to the one-dimensional quartic anharmonic oscillator by Turchetti³ and then studied rigorously by Graffi and Paul.⁴ (The most important features of this classical limit are summarized in Appendix A.)

In this paper we focus on time dependent quantum mechanical perturbation theory with the same goal in mind, i.e. retrieving classical mechanical perturbation expansions from their QM counterparts by means of an appropriate classical limit which involves the mathematical operation $\hbar \rightarrow 0$. Here we explore in some detail a perturbation method introduced by Bhaumik and Dutta-Roy (BD)⁵ which involves harmonic oscillator coherent states (HOCS) $|\alpha\rangle$, where $\alpha \in \mathbb{C}$. As is well known,^{6–8} in the time evolution of a HOCS under the harmonic oscillator Hamiltonian, the quantum expectation value $\langle x(t) \rangle$ becomes the classical function $x(t) = A \cos(\omega_0 t + \phi)$ when the following classical limit is taken: $\hbar \rightarrow 0, |\alpha| \rightarrow \infty$, with $|\alpha|/\sqrt{\hbar}$ fixed and proportional to A . BD applied this classical limit of coherent states (which we refer to as CLCS) to the time dependent quantum mechanical perturbation expansion for an anharmonic oscillator where the initial condition $\Psi(x, 0)$ was a perturbed HOCS. It was observed that in this classical limit the perturbation expansion for $\langle \Psi(x, t) | \hat{x} | \Psi(x, t) \rangle$ becomes, at least to first order, the Poincaré–Lindstedt perturbation series for the position $x(t)$ of the periodic orbit for the classical anharmonic oscillator. [Here, $\Psi(x, t)$ is the solution of the time dependent Schrödinger equation for the anharmonic potential.] Subsequently, the BD perturbation method was applied to a variety of Hamiltonians^{9–17} and the classical perturbation series retrieved in all cases. However, all calculations, including those of BD, were performed only to first order. In a number of papers, it was concluded that the

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extension of this perturbation method and its classical limit would be straightforward. Indeed, in a somewhat cavalier fashion, it was also suggested that this procedure could actually represent an easier method to generate the well known classical perturbation expansions for periodic orbits. We have found that this is *not* the case. Indeed, a proper calculation of even the second order quantum corrections involves a great deal of care and the extension to higher orders is not obvious. The quantum results involve infinite summations which can be written in closed form only if first order terms are retained, but cannot be expressed in closed form if higher order terms are included. In addition, the success of this method depends heavily upon the initial conditions chosen for the quantum problem. We show below that “secular terms” in the classical limit of the quantum expansions are avoided if the initial conditions specified by BD are chosen. The proper classical mechanical expansions may be obtained (at least to second order), but only if a proper “renormalization” of expansions is performed. This is actually analogous to what happens in classical mechanics, as we explain below. Preliminary results¹⁸ and later progress¹⁹ of this procedure have been reported. Complete details are to be found in the thesis of McRae.²⁰

The complications in higher order calculations mentioned above are not limited to perturbation theory in the Schrödinger picture—they also appear in the Heisenberg picture. We have also studied this problem and refer the reader to Ref. 21 for details.

We conclude this paper by establishing a connection between the $n\hbar = J$ classical limit of time independent (Rayleigh–Schrödinger) perturbation theory and the $|\alpha|\sqrt{\hbar}$ classical limit of time dependent coherent state perturbation theory. The connection between these two limits is not obvious apart from the common mathematical operation of letting $\hbar \rightarrow 0$. Some insight is provided from an analysis of the unperturbed harmonic oscillator problem. This connection between limits also reveals that an infinity of quantum mechanical wavefunctions contribute to the construction of a single classical orbit in the classical limit.

Many of the calculations presented in this paper were done with the aid of the symbolic computation package MAPLE.^{22,23}

II. CLASSICAL PERTURBATION THEORY: ESSENTIALS

Of specific interest are periodic solutions $(x(t), p(t))$ to Hamilton’s equations of motion, $\dot{x}(t) = \partial H / \partial p$ and $\dot{p}(t) = -\partial H / \partial x$, in particular, where the Hamiltonian function $H(x, p)$ is the perturbation of a solvable problem,

$$H(x, p) = H^{(0)}(x, p) + \lambda H^{(1)}(x, p). \quad (2.1)$$

A standard technique for determining periodic orbits of such perturbed problems is the Poincaré–Lindstedt method (see Nayfeh²⁴ p. 58, Murdock²⁵ p. 157, or Verhulst²⁶ p. 130, for example). It is normally applied to problems having the form

$$\ddot{x} + \omega_0^2 x = \varepsilon f(t, x, \dot{x}, \varepsilon), \quad (2.2)$$

where f either does not depend explicitly upon t (i.e., an autonomous system) or is periodic in t . The key idea of this method is that a T -periodic solution to Eq. (2.2) is written as a generalized asymptotic expansion of the form

$$x(t) = \sum_{n=0}^N x_n(s) \varepsilon^n + O(\varepsilon^{N+1}), \quad \text{as } \varepsilon \rightarrow 0, \quad (2.3)$$

where the perturbation coefficients $x_k(s)$ are T -periodic in the scaled time variable $s = \omega t$. The frequency ω is expressed as an asymptotic expansion in powers ε , i.e.

$$\omega = \omega_0 + \omega_1 \varepsilon + \omega_2 \varepsilon^2 + \cdots. \quad (2.4)$$

The corrections ω_k are typically determined by the requirement that no secular, or unbounded, solutions (e.g., $t \sin \omega_0 t$) may appear. Details of this procedure and applications may be found in the references cited above.

We shall be primarily concerned with the quartic anharmonic oscillator Hamiltonian,

$$H(x, p) = \frac{p^2}{2m} + \frac{m\omega_0^2}{2} x^2 + \lambda x^4. \quad (2.5)$$

From Hamilton's equations we have

$$\ddot{x} + \omega_0^2 x + \varepsilon x^3 = 0, \quad (2.6)$$

where $\varepsilon = 4\lambda m^{-1}$. Now assume that the initial conditions are given by

$$x(0) = A, \quad \dot{x}(0) = 0. \quad (2.7)$$

The net result, to second order in λ , is

$$\begin{aligned} x(t) = & A \cos(\omega t) + \frac{A^3 \lambda}{8m\omega_0^2} [\cos(3\omega t) - \cos(\omega t)] + \frac{A^5 \lambda^2}{16\omega_0^4 m^2} \\ & \times \left[\frac{23}{4} \cos(\omega t) - 6 \cos(3\omega t) + \frac{1}{4} \cos(5\omega t) \right] + \cdots, \end{aligned} \quad (2.8)$$

where

$$\omega = \omega_0 + \frac{3A^2}{2m\omega_0} \lambda - \frac{21A^4}{16m^2\omega_0^3} \lambda^2 + \frac{81A^6}{32m^3\omega_0^5} \lambda^3 + \cdots. \quad (2.9)$$

The perturbation expansion for the momentum can be found by differentiating Eq. (2.8):

$$\begin{aligned} p(t) = m\dot{x}(t) = & -m\omega_0 A \sin(\omega t) + \frac{A^3 \lambda}{8\omega_0} [-11 \sin(\omega t) - 3 \sin(3\omega t)] \\ & + \frac{A^5 \lambda^2}{64m\omega_0^3} [73 \sin(\omega t) + 36 \sin(3\omega t) - 5 \sin(5\omega t)] + \cdots. \end{aligned} \quad (2.10)$$

From Eq. (2.9), the frequency ω depends upon the amplitude of oscillation A , a behavior characteristic of nonlinear oscillations. *We are particularly interested in how such nonlinear features emerge from "linear" quantum mechanics as $\hbar \rightarrow 0$.*

Finally, it is extremely important to note that the Poincaré–Lindstedt perturbation expansions are sensitive to the initial conditions assumed for the problem. For example, the expansions in Eqs. (2.8) and (2.9) arise from the rather standard initial conditions of Eq. (2.7). However, a look at Nayfeh,²⁴ for example, reveals a slightly different expansion—the second order correction in the frequency has (apart from normalization) a numerical factor of $\frac{15}{16}$ instead of $\frac{21}{16}$. In Nayfeh,²⁴ a different set of initial conditions was imposed. One can make a correspondence between the two expansions with a proper “renormalization” of the amplitude of oscillation, as we now briefly show. This is a rather important feature that has been ignored in a number of papers, especially when the results are compared to references such as Nayfeh.²⁴

In Nayfeh's approach, the initial conditions for each $x_k(s)$ in Eq. (2.3) are chosen so that the characteristic solution for each differential equation in the hierarchy is zero. Note that in the resulting solutions,

$$\begin{aligned}\tilde{x}(t) = & \mathcal{A} \cos(\tilde{\omega}t + \varphi) + \frac{\mathcal{A}^3 \lambda}{8\omega_0^2 m} \cos[3(\tilde{\omega}t + \varphi)] \\ & + \frac{\mathcal{A}^5 \lambda^2}{64\omega_0^4 m^2} \{-21 \cos[3(\tilde{\omega}t + \varphi)] + \cos[5(\tilde{\omega}t + \varphi)]\} + \dots,\end{aligned}\quad (2.11)$$

$$\tilde{\omega} = \omega_0 + \frac{3\mathcal{A}^2 \lambda}{2m\omega_0} - \frac{15\mathcal{A}^4 \lambda^2}{16m^2 \omega_0^3} + \dots, \quad (2.12)$$

the initial condition $\tilde{x}(0)$ is a series in λ . By setting $\varphi=0$ and inverting the series

$$A = \mathcal{A} + \frac{\mathcal{A}^3 \lambda}{8\omega_0^2 m} - \frac{5\mathcal{A}^5 \lambda^2}{16\omega_0^4 m^2} + \dots, \quad (2.13)$$

one can recover the solutions in Eqs. (2.8) and (2.9).

We show below that quantum mechanical expansions will also demonstrate such a phenomenon with respect to initial conditions.

III. QM TIME DEPENDENT PERTURBATION THEORY

We now consider the quantum mechanical counterpart of the previous section, namely, the time evolution of quantum states under the influence of perturbed Hamiltonians, as determined by the time dependent Schrödinger equation (TDSE),

$$i\hbar \frac{\partial \Psi}{\partial t}(x, t) = \hat{H} \Psi(x, t), \quad (3.1)$$

where

$$\hat{H} = \hat{H}^{(0)} + \lambda \hat{H}^{(1)}. \quad (3.2)$$

As usual, it is assumed that the eigenvalues and eigenfunctions of the unperturbed time independent Schrödinger equation are known:

$$\hat{H}^{(0)} \phi_n^{(0)} = E_n^{(0)} \phi_n^{(0)}, \quad n = 0, 1, \dots \quad (3.3)$$

Let the time independent Schrödinger equation for the Hamiltonian in Eq. (3.2) be denoted by

$$\hat{H} \phi_n = E_n \phi_n, \quad n = 0, 1, 2, \dots \quad (3.4)$$

Our focus will be the QM counterpart to Eq. (2.5), namely, the QM quartic anharmonic oscillator, with Hamiltonian

$$\hat{H}(\hat{x}, \hat{p}) = \frac{\hat{p}^2}{2m} + \frac{m\omega_0^2}{2} \hat{x}^2 + \lambda \hat{x}^4. \quad (3.5)$$

There are two major concerns in the formulation of a perturbation method.

(1) **The basis set:** The usual procedure in the Schrödinger picture is to assume a perturbation expansion for the wavefunction $\Psi(x, t)$ in terms of the *unperturbed* eigenfunctions $\phi_n^{(0)}(x)$ of $\hat{H}^{(0)}$. As in classical perturbation theory, however, there is a price to pay, namely, the appearance of secular terms. Dirac's²⁷⁻³⁰ variation of constants method is the most common approach to

removing secular terms from perturbation expansions in the unperturbed basis. Langhoff *et al.*³¹ have clarified certain aspects of the Dirac method such as how to deal properly with secular and normalization terms at higher orders, but their methods are developed only for situations where the initial condition is a single unperturbed eigenfunction. Bhattacharyya^{32,33} introduced an undetermined phase method which can be adapted to handle more complicated initial conditions. This method provides the same result as the BD method. The method of Bhaumik and Dutta-Roy, i.e. assuming an expansion in the eigenfunctions $\phi_n(x)$ of the perturbed Hamiltonian $\hat{H} = \hat{H}^{(0)} + \lambda \hat{H}^{(1)}$, essentially bypasses the problem of secular terms. If the initial condition of Eq. (3.1) may be written as

$$\Psi(x,0) = \sum_{n=0}^{\infty} C_n \phi_n(x), \quad (3.6)$$

then its time evolution in the “diagonal” basis $\{\phi_n\}$ is given simply by

$$\Psi(x,t) = \sum_{n=0}^{\infty} C_n e^{-iE_n t/\hbar} \phi_n(x). \quad (3.7)$$

This formulation may be considered as a kind of scaling of time, roughly analogous to the Poincaré–Lindstedt method of classical mechanics.

(2) **The initial condition $\Psi(x,0)$:** The goal is to produce dynamical quantum states whose classical limits yield periodic orbits in x - p phase space. This rules out the use of eigenstates, whose time evolution involves only a change in phase. Instead, it is more natural to consider the harmonic oscillator coherent states (HOCS), which are dynamical states of the unperturbed harmonic oscillator. The HOCS are defined as^{6–8,34–40}

$$|\alpha\rangle = e^{-|\alpha|^2/2} \sum_{n=0}^{\infty} \frac{\alpha^n}{\sqrt{n!}} \phi_n^{(0)}(x), \quad (3.8)$$

where the $\phi_n^{(0)}(x)$ denote the harmonic oscillator eigenfunctions and $\alpha \in \mathbf{C}$. If $\Psi(x,0) = |\alpha\rangle$ in Eq. (3.1) and \hat{H} is the Hamiltonian for the harmonic oscillator, then

$$\Psi^{(0)}(x,t) = e^{-i\omega_0 t/2} |\alpha e^{-i\omega_0 t}\rangle. \quad (3.9)$$

In other words, a HOCS remains a HOCS. From

$$\langle \Psi^{(0)}(x,t) | \hat{x} | \Psi^{(0)}(x,t) \rangle = \sqrt{\frac{2\hbar}{m\omega_0}} |\alpha| \cos(\omega_0 t + \varphi), \quad (3.10)$$

where $\alpha = |\alpha| e^{-i\varphi}$, and the classical harmonic oscillator solution $x(t) = A \cos(\omega_0 t + \varphi)$, one may define the following classical limit for coherent states (CLCS):

$$\text{CLCS: } \lim_{|\alpha| \rightarrow \infty, \hbar \rightarrow 0} |\alpha|^2 = \gamma \equiv \frac{m\omega_0}{2} A^2. \quad (3.11)$$

It also follows that

$$\lim_{CLCS} |\Psi^{(0)}(x,t)|^2 = \delta[x - A \cos(\omega_0 t + \varphi)], \quad (3.12)$$

where $\delta(x)$ denotes the Dirac delta function. An analogous result holds for momentum.

Bhaumik and Dutta-Roy⁵ employed the CLCS to study the TDSE for perturbed harmonic oscillator problems using coherent states. Their method may be summarized as follows.

(1) Assume the following initial condition for the TDSE in Eq. (3.1):

$$\Psi(x,0) = |\alpha\rangle' = e^{-|\alpha|^2/2} \sum_{n=0}^{\infty} \frac{\alpha^n}{\sqrt{n!}} \phi_n(x), \quad (3.13)$$

where the $\phi_n(x)$ denote the solutions to the *perturbed* harmonic oscillator eigenvalue problem given in Eq. (3.4).

- (2) Solve the TDSE for $\Psi(x,t)$ as a perturbation series in λ . This is relatively straightforward in the diagonal ϕ_n basis.
- (3) Apply the CLCS to the the perturbation expansion for the quantum expectation value $\langle x \rangle(t) = \langle \Psi(x,t) | \hat{x} | \Psi(x,t) \rangle$ to produce a perturbation series $\langle x \rangle_{CLCS}(t)$.

BD performed the above calculation, but only to first order. It was observed that the perturbation series $\langle x \rangle_{CLCS}(t)$ agreed with the Poincaré–Lindstedt series for $x(t)$ for the corresponding perturbed classical problem. However, as we show below, both the calculation of second and higher order terms and their comparison with classical expansions must be done with extreme care. There are two major points.

- (1) Secular terms are avoided in the BD method.
- (2) Since the initial conditions of this problem do not involve an unperturbed coherent state, higher order terms do *not* agree (in the classical limit) with the expansion in Eqs. (2.8) and (2.9), in particular, with regard to the perturbation series for the frequency $\omega(\lambda)$.

In order to better understand the nature of the classical limit of such time dependent quantum perturbation expansions, we have examined this perturbation method in the perturbed oscillator basis using *two* different sets of initial conditions, which we refer to as follows.

Method 1: The initial condition is the exact HOCS $|\alpha\rangle$ in Eq. (3.8),

Method 2: The initial condition used by BD; a kind of perturbed HOCS $|\alpha\rangle'$ in Eq. (3.13).

Method 1 would seem to be the natural choice since one starts with a HOCS with a well defined classical limit/amplitude. It will be seen, however, that Method 2 is a far more convenient way to both calculate the perturbation expansion for $\langle x \rangle(t)$ and take its classical limit. In both cases, it is useful to employ a set of perturbed eigenfunctions ϕ_n of \hat{H} which satisfy the *orthonormalization* condition $\langle \phi_m | \phi_n \rangle = \delta_{m,n}$ rather than the *intermediate normalization* condition $\langle \phi_n^{(0)} | \phi_n \rangle = 1$ when constructing the RS perturbation expansions. Details of these two different normalization conditions are given by Hirschfelder *et al.*⁴¹ (Note: This important point did not have to be considered by BD since both normalization methods give the same results to first order.)

A. Method 1: HOCS initial condition

Using the initial condition of Eq. (3.8) and the expansion of Eq. (3.6) and the fact that $\langle \phi_k | \phi_n \rangle = \delta_{kn}$ we have

$$C_n = e^{-|\alpha|^2/2} \sum_{k=0}^{\infty} \frac{\alpha^k}{\sqrt{k!}} \langle \phi_n | \phi_k^{(0)} \rangle. \quad (3.14)$$

Using Eq. (3.7)

$$\langle \Psi(x,t) | \hat{a} | \Psi(x,t) \rangle = \sum_{n=0}^{\infty} \sum_{m=0}^{\infty} C_n C_m^* \exp \left[\frac{it}{\hbar} (E_m - E_n) \right] \langle \phi_m | \hat{a} | \phi_n \rangle, \quad (3.15)$$

where \hat{a} is the annihilation operator:

$$\hat{a} = \frac{1}{\sqrt{2m\hbar\omega_0}}(m\omega_0\hat{x} + i\hat{p}). \quad (3.16)$$

Now, the method will be applied to the quartic anharmonic oscillator whose Hamiltonian is given by Eq. (3.5). The (time independent) Rayleigh Schrödinger perturbation theory (RSPT) expansions in λ for the eigenvalue E_n and the eigenvector ϕ_n are first constructed:

$$E_n = E_n^{(0)} + E_n^{(1)}\lambda + E_n^{(2)}\lambda^2 + O(\lambda^3), \quad (3.17)$$

$$\phi_n = \phi_n^{(0)} + \phi_n^{(1)}\lambda + \phi_n^{(2)}\lambda^2 + O(\lambda^3). \quad (3.18)$$

For future reference,

$$E_n^{(0)} = \hbar\omega_0(n + 1/2), \quad (3.19)$$

$$E_n^{(1)} = \frac{3\hbar^2}{4m^2\omega_0^2}(2n^2 + 2n + 1), \quad (3.20)$$

$$E_n^{(2)} = -\frac{\hbar^3}{m^4\omega_0^5}\left(\frac{17}{4}n^3 + \frac{51}{8}n^2 + \frac{59}{8}n + \frac{21}{8}\right), \quad (3.21)$$

$$E_n^{(3)} = \frac{\hbar^4}{2m^6\omega_0^8}\left(\frac{375}{8}n^4 + \frac{375}{4}n^3 + 177n^2 + \frac{1041}{8}n + \frac{333}{8}\right), \quad (3.22)$$

$$\begin{aligned} \phi_n^{(1)} = & \frac{\hbar}{4m^2\omega_0^3}\left[\frac{1}{4}\sqrt{n(n-1)(n-2)(n-3)}\phi_{n-4}^{(0)} + (2n-1)\sqrt{n(n-1)}\phi_{n-2}^{(0)} \right. \\ & - (2n+3)\sqrt{(n+1)(n+2)}\phi_{n+2}^{(0)} \\ & \left. - \frac{1}{4}\sqrt{(n+1)(n+2)(n+3)(n+4)}\phi_{n+4}^{(0)}\right], \end{aligned} \quad (3.23)$$

and

$$\begin{aligned} \phi_n^{(2)} = & \frac{\hbar^2}{16m^4\omega_0^6}\left[\frac{1}{32}\sqrt{n(n-1)\cdots(n-7)}\phi_{n-8}^{(0)} \right. \\ & + \frac{1}{12}(6n-11)\sqrt{n(n-1)\cdots(n-5)}\phi_{n-6}^{(0)} \\ & + (2n^2-9n+7)\sqrt{n(n-1)(n-2)(n-3)}\phi_{n-4}^{(0)} \\ & - \frac{1}{4}(2n^3+129n^2-107n+66)\sqrt{n(n-1)}\phi_{n-2}^{(0)} \\ & \left. - \frac{1}{16}(65n^4+130n^3+487n^2+422n+156)\phi_n^{(0)}\right] \end{aligned}$$

$$\begin{aligned}
& -\frac{1}{4}(2n^3 - 123n^2 - 359n - 300)\sqrt{(n+1)(n+2)}\phi_{n+2}^{(0)} \\
& + (2n^2 + 13n + 18)\sqrt{(n+1)\cdots(n+4)}\phi_{n+4}^{(0)} \\
& + \frac{1}{12}(6n + 17)\sqrt{(n+1)\cdots(n+6)}\phi_{n+6}^{(0)} \\
& + \frac{1}{32}\sqrt{(n+1)\cdots(n+8)}\phi_{n+8}^{(0)} \Big]. \tag{3.24}
\end{aligned}$$

Using the notation

$$C_n = C_n^{(0)} + \lambda C_n^{(1)} + \lambda^2 C_n^{(2)} + O(\lambda^3), \tag{3.25}$$

and substituting Eq. (3.18) into Eq. (3.15) yields

$$\langle \Psi(x, t) | \hat{a} | \Psi(x, t) \rangle = S1 + \lambda(S2 + S3) + \lambda^2(S4 + S5 + S6) + O(\lambda^3), \tag{3.26}$$

where

$$S1 = \sum_{n=0}^{\infty} \sum_{m=0}^{\infty} \exp\left[\frac{it}{\hbar}(E_m - E_n)\right] C_n^{(0)} C_m^{*(0)} \langle \phi_m^{(0)} | \hat{a} | \phi_n^{(0)} \rangle, \tag{3.27}$$

$$S2 = \sum_{n=0}^{\infty} \sum_{m=0}^{\infty} \exp\left[\frac{it}{\hbar}(E_m - E_n)\right] (C_n^{(0)} C_m^{*(1)} + C_n^{(1)} C_m^{*(0)}) \langle \phi_m^{(0)} | \hat{a} | \phi_n^{(0)} \rangle, \tag{3.28}$$

$$S3 = \sum_{n=0}^{\infty} \sum_{m=0}^{\infty} \exp\left[\frac{it}{\hbar}(E_m - E_n)\right] C_n^{(0)} C_m^{*(0)} (\langle \phi_m^{(0)} | \hat{a} | \phi_n^{(1)} \rangle + \langle \phi_m^{(1)} | \hat{a} | \phi_n^{(0)} \rangle), \tag{3.29}$$

$$S4 = \sum_{n=0}^{\infty} \sum_{m=0}^{\infty} \exp\left[\frac{it}{\hbar}(E_m - E_n)\right] (C_n^{(2)} C_m^{*(0)} + C_n^{(1)} C_m^{*(1)} + C_n^{(0)} C_m^{*(2)}) \langle \phi_m^{(0)} | \hat{a} | \phi_n^{(0)} \rangle, \tag{3.30}$$

$$S5 = \sum_{n=0}^{\infty} \sum_{m=0}^{\infty} \exp\left[\frac{it}{\hbar}(E_m - E_n)\right] C_n^{(0)} C_m^{*(0)} (\langle \phi_m^{(0)} | \hat{a} | \phi_n^{(2)} \rangle + \langle \phi_m^{(1)} | \hat{a} | \phi_n^{(1)} \rangle + \langle \phi_m^{(2)} | \hat{a} | \phi_n^{(0)} \rangle), \tag{3.31}$$

and

$$\begin{aligned}
S6 = & \sum_{n,m=0}^{\infty} \exp\left[\frac{it}{\hbar}(E_m - E_n)\right] (C_n^{(1)} C_m^{*(0)} + C_n^{(0)} C_m^{*(1)}) \\
& \times (\langle \phi_m^{(0)} | \hat{a} | \phi_n^{(1)} \rangle + \langle \phi_m^{(1)} | \hat{a} | \phi_n^{(0)} \rangle). \tag{3.32}
\end{aligned}$$

We now wish to rearrange these expansions in order to facilitate the application of the classical limit. First consider the zeroth order term $S1$. Using properties of the annihilation operator acting on the harmonic oscillator wave function, we have

$$\langle \phi_m^{(0)} | \hat{a} | \phi_n^{(0)} \rangle = \sqrt{n} \delta_{m,n-1}. \quad (3.33)$$

From Eqs. (3.14), (3.18), and (3.25),

$$C_n^{(0)} = e^{-|\alpha|^2/2} \frac{\alpha^n}{\sqrt{n!}}. \quad (3.34)$$

The zeroth order term then becomes

$$S1 = \alpha e^{-|\alpha|^2} \sum_{n=0}^{\infty} \frac{|\alpha|^{2n}}{n!} \exp \left[\frac{it}{\hbar} (E_n - E_{n+1}) \right]. \quad (3.35)$$

The discussion of the classical limit of this expression will be deferred until later.

Consider the first order expressions. From Eqs. (3.14), (3.18), (3.23), (3.25), (3.33), and (3.34) we have

$$\begin{aligned} S2 = & \frac{\hbar}{4m^2\omega_0^3} e^{-|\alpha|^2} \left\{ \frac{\alpha^5}{4} \sum_{n=0}^{\infty} \exp \left[\frac{it}{\hbar} (E_{n+4} - E_{n+5}) \right] \frac{|\alpha|^{2n}}{n!} \right. \\ & + \alpha^3 \sum_{n=0}^{\infty} \exp \left[\frac{it}{\hbar} (E_{n+2} - E_{n+3}) \right] \frac{|\alpha|^{2n}}{n!} (2n+3) \\ & - \alpha(\alpha^*)^2 \sum_{n=0}^{\infty} \exp \left[\frac{it}{\hbar} (E_n - E_{n+1}) \right] \frac{|\alpha|^{2n}}{n!} (2n+3) \\ & - \frac{\alpha(\alpha^*)^4}{4} \sum_{n=0}^{\infty} \exp \left[\frac{it}{\hbar} (E_n - E_{n+1}) \right] \frac{|\alpha|^{2n}}{n!} \\ & + \frac{(\alpha^*)^3}{4} \sum_{n=0}^{\infty} \exp \left[\frac{it}{\hbar} (E_{n+3} - E_{n+4}) \right] \frac{|\alpha|^{2n}}{n!} (n+4) \\ & + \alpha^* \sum_{n=0}^{\infty} \exp \left[\frac{it}{\hbar} (E_{n+1} - E_{n+2}) \right] \frac{|\alpha|^{2n}}{n!} (2n^2 + 7n + 6) \\ & - \alpha^3 \sum_{n=0}^{\infty} \exp \left[\frac{it}{\hbar} (E_n - E_{n+1}) \right] \frac{|\alpha|^{2n}}{n!} (2n+5) \\ & \left. - \frac{\alpha^5}{4} \sum_{n=0}^{\infty} \exp \left[\frac{it}{\hbar} (E_n - E_{n+1}) \right] \frac{|\alpha|^{2n}}{n!} \right\}. \quad (3.36) \end{aligned}$$

It is difficult to take the classical limit of the above expression. Equation (B2) can be used to cast Eq. (3.36) in a form that is more amenable to taking the classical limit. Since α is a complex number, let $\alpha = |\alpha| e^{-i\varphi}$. In order to ensure that the quantum initial conditions correspond to the classical initial conditions given in Eq. (2.7), we require that $\varphi=0$ [see Eq. (3.10) and Section III C]. Since it simplifies the results, we will replace α with $|\alpha|$ at this point. The simplified version of Eq. (3.36) is

$$\begin{aligned} S2 = & \frac{\hbar}{4m^2\omega_0^3} e^{-|\alpha|^2} \left\{ \left[\frac{1}{2} (T_{4,5} - T_{0,1}) + 4(T_{3,4} - T_{1,2}) \right] |\alpha|^5 \right. \\ & \left. + [-8T_{0,1} + 12T_{2,3} + T_{3,4}] |\alpha|^3 + 6T_{1,2} |\alpha| \right\}, \quad (3.37) \end{aligned}$$

where

$$T_{j,k} = \sum_{n=0}^{\infty} \frac{|\alpha|^{2n}}{n!} \exp\left[\frac{it(E_{n+j} - E_{n+k})}{\hbar}\right]. \quad (3.38)$$

After performing similar simplifications on the other terms, we obtain

$$S3 = \frac{\hbar}{4m^2\omega_0^3} e^{-|\alpha|^2} \{|\alpha|^3 [2T_{0,3} - 6T_{2,1} - T_{3,0}] - 6|\alpha|T_{1,0}\}, \quad (3.39)$$

$$\begin{aligned} S4 = e^{-|\alpha|^2} \frac{\hbar^2}{16m^4\omega_0^6} & \{[\frac{1}{8}(T_{0,1} + T_{8,9} - 2T_{4,5}) + 2(T_{1,2} + T_{7,8} - 2T_{4,5}) \\ & + 8(T_{2,3} + T_{6,7} - 2T_{4,5}) - 2(T_{3,4} + T_{5,6} - 2T_{4,5})] \\ & \times |\alpha|^9 + [\frac{16}{3}(T_{0,1} - T_{3,4}) + 54(T_{1,2} - T_{3,4}) + 54(T_{2,3} - T_{4,5}) + 90(T_{5,6} - T_{3,4}) + \frac{74}{3}(T_{6,7} - T_{4,5}) \\ & + \frac{3}{2}(T_{7,8} - T_{3,4}) + \frac{16}{3}(T_{3,4} - T_{4,5})]|\alpha|^7 + [66T_{0,1} + 297T_{1,2} - 366T_{2,3} - 444T_{3,4} + 306T_{4,5} \\ & + 95T_{5,6} + \frac{15}{2}T_{6,7}]|\alpha|^5 + [270T_{0,1} - \frac{669}{2}T_{1,2} - 624T_{2,3} + 342T_{3,4} + 120T_{4,5} + 15T_{5,6}]|\alpha|^3 \\ & + [-\frac{177}{2}T_{0,1} - 192T_{1,2} + 90T_{2,3} + 30T_{3,4} + \frac{15}{2}T_{4,5}]|\alpha|\}, \end{aligned} \quad (3.40)$$

$$\begin{aligned} S5 = e^{-|\alpha|^2} \frac{\hbar^2}{16m^4\omega_0^6} & \{[3T_{0,5} - 2T_{5,0} - 60T_{1,4} + 21T_{4,1} + \frac{27}{2}T_{2,3} + 138T_{3,2}]|\alpha|^5 \\ & + [-120T_{0,3} + 42T_{3,0} + \frac{81}{2}T_{1,2} + 414T_{2,1}]|\alpha|^3 + [9T_{0,1} + 180T_{1,0}]|\alpha|\}, \end{aligned} \quad (3.41)$$

and

$$\begin{aligned} S6 = e^{-|\alpha|^2} \frac{\hbar^2}{16m^4\omega_0^6} & \{[(T_{4,7} - T_{0,3}) + \frac{1}{2}(T_{3,0} - T_{7,4}) + 3(T_{2,1} - T_{6,5}) + 8(T_{3,6} - T_{1,4}) + 4(T_{4,1} - T_{6,3}) \\ & + 24(T_{3,2} - T_{5,4})]|\alpha|^7 + [3T_{1,0} + 96T_{2,1} - 24T_{0,3} + 12T_{3,0} + 48T_{2,5} - 24T_{5,2} - 168T_{4,3} + 6T_{3,6} \\ & - 3T_{6,3} - 21T_{5,4}]|\alpha|^5 + [48T_{1,0} + 108T_{1,4} - 54T_{4,1} - 252T_{3,2} + 18T_{2,5} - 9T_{5,2} - 24T_{4,3}]|\alpha|^3 \\ & + [60T_{0,3} - 30T_{3,0} - 72T_{2,1} + 12T_{1,4} - 6T_{4,1}]|\alpha|\}. \end{aligned} \quad (3.42)$$

We have now accounted for all terms in the asymptotic expansion of Eq. (3.26). For a more detailed account of these calculations, we refer the reader to the thesis of McRae.²⁰

B. Method 2: Perturbed HOCS initial condition (BD)

As stated earlier, the initial condition used by BD is

$$\Phi(x,0) = e^{-|\alpha|^2/2} \sum_{n=0}^{\infty} \frac{\alpha^n}{\sqrt{n!}} \phi_n. \quad (3.43)$$

Assuming the expansion

$$\Phi(x, t) = \sum_{n=0}^{\infty} \mathcal{E}_n \exp\left(-\frac{iE_n t}{\hbar}\right) \phi_n(x), \quad (3.44)$$

we have

$$\langle \Phi(x, t) | \hat{a} | \Phi(x, t) \rangle = \sum_{n=0}^{\infty} \sum_{m=0}^{\infty} \mathcal{E}_n \mathcal{E}_m^* \exp\left[\frac{it}{\hbar}(E_m - E_n)\right] \langle \phi_m | \hat{a} | \phi_n \rangle, \quad (3.45)$$

where

$$\mathcal{E}_n = e^{-|\alpha|^2/2} \frac{\alpha^n}{\sqrt{n!}}. \quad (3.46)$$

Obviously, the expression for \mathcal{E}_n much simpler than that of C_n in Method 1, cf. Eq. (3.14). The solution of Method 2 is comprised of the $S1$, $S3$, and $S5$ terms of Method 1.

C. Classical Limit of Method 1

For the sake of notation, let

$$\langle \Psi(x, t) | \hat{x} | \Psi(x, t) \rangle = \sum_{n=0}^{\infty} \langle \hat{x} \rangle^{(n)} \lambda^n. \quad (3.47)$$

Using Eq. (3.26) and the fact that

$$\hat{x} = \sqrt{\frac{\hbar}{2m\omega_0}} (\hat{a} + \hat{a}^\dagger), \quad (3.48)$$

the zeroth order term is given by

$$\langle \hat{x} \rangle^{(0)} = \sqrt{\frac{\hbar}{2m\omega_0}} (S1 + S1^*). \quad (3.49)$$

Setting $\alpha = |\alpha| e^{-i\varphi}$ and using Eqs. (3.11), (3.35), and (B8), it follows that

$$\lim_{CLCS} \langle \hat{x} \rangle^{(0)} = A \cos(Wt + \varphi), \quad (3.50)$$

where the frequency W admits the series expansion given in Eq. (B9).

At this point, we can note two discrepancies from the zeroth order classical solution given in Eqs. (2.8) and (2.9).

- (1) There is no phase term in the classical solution [due to the initial conditions in Eq. (2.7)]. This can be easily remedied by setting $\varphi = 0$ in the quantum result.
- (2) The frequency expansion in Eq. (B9) does *not* agree with the classical frequency expansion of Eq. (2.9), specifically as regards the second order term. The explanation for this observation is a bit more subtle.

Consider the zeroth order term from the classical Poincaré–Lindstedt method, $A \cos(\omega t)$. From Eqs. (2.9) and (B9), we can write the classical Poincaré–Lindstedt frequency as

$$\omega = W + \frac{15A^4\lambda^2}{8m^2\omega_0^3} - \frac{147A^6\lambda^3}{16m^3\omega_0^5} + \dots \quad (3.51)$$

Writing the classical Poincaré–Lindstedt solution for $x(t)$ given in Eq. (2.8) in terms of W and replacing other trigonometric functions with the first few terms of their Taylor series expansions,

$$\begin{aligned} x(t) = & A \cos(Wt) + \frac{A^3\lambda}{8m\omega_0^2} [\cos(3Wt) - \cos(Wt)] - \frac{15A^5\lambda^2 t}{8m^2\omega_0^3} \sin(Wt) \\ & + \frac{A^5\lambda^2}{16m^2\omega_0^4} \left[\frac{23}{4} \cos(Wt) - 6 \cos(3Wt) + \frac{1}{4} \cos(5Wt) \right] \\ & + \frac{A^7\lambda^3 t}{64m^3\omega_0^5} [603 \sin(Wt) - 45 \sin(3Wt)] \\ & - \frac{225A^9\lambda^4 t^2}{128m^4\omega_0^6} \cos(Wt) + O(\lambda^4). \end{aligned} \quad (3.52)$$

Thus, in order for the classical limit of the BD method to agree with the classical Poincaré–Lindstedt results, secular terms must arise from the classical limit of higher order terms in the quantum BD series. This turns out to be the case, as we now show.

Consider the classical limit of the first order terms in Eq. (3.47):

$$\langle \hat{x} \rangle^{(1)} = \sqrt{\frac{\hbar}{2m\omega_0}} (S_2 + S_2^* + S_3 + S_3^*). \quad (3.53)$$

Using Eqs. (3.37) and (3.39),

$$\begin{aligned} \langle \hat{x} \rangle^{(1)} = & \sqrt{\frac{\hbar^3}{32m^5\omega_0^7}} e^{-|\alpha|^2} \left\{ \left[\frac{1}{2} (T_{4,5} - T_{0,1}) + 4(T_{3,4} - T_{1,2}) \right] |\alpha|^5 \right. \\ & + [-8T_{0,1} + 12T_{2,3} + T_{3,4} + 2T_{0,3} - 6T_{2,1} - T_{3,0}] |\alpha|^3 \\ & \left. + 6[T_{1,2} - T_{1,0}] |\alpha| \right\} + \text{complex conjugate}. \end{aligned} \quad (3.54)$$

In order to calculate the classical limit of the $|\alpha|^5$ term, we must use the results given in Eqs. (B11) and (B12). The classical limit of the other terms can be obtained with the use of Eq. (B8). The result is

$$\lim_{CLCS} \langle \hat{x} \rangle^{(1)} = \frac{A^3}{8m\omega_0^2} [\cos(3Wt) - \cos(Wt) - 20t\sigma \sin(Wt)], \quad (3.55)$$

where σ is given by Eq. (B12). Explicitly writing out the first few terms of σ , we have

$$\lim_{CLCS} \lambda \langle \hat{x} \rangle^{(1)} = \frac{A^3\lambda}{8m\omega_0^2} [\cos(3Wt) - \cos(Wt)] - \frac{15A^5\lambda^2 t}{8m^2\omega_0^3} \sin(Wt) + \frac{255A^7\lambda^3 t}{32m^3\omega_0^5} \sin(Wt) + O(\lambda^4). \quad (3.56)$$

Note that the first term in σ gives the order λ^2 secular term that was predicted in Eq. (3.52) by rearranging the classical solution.

Now consider the classical limit of the second order terms [see Eqs. (3.40), (3.41), and (3.42)]:

$$\langle \hat{x} \rangle^{(2)} = \sqrt{\frac{\hbar}{2m\omega_0}} (S4 + S4^* + S5 + S5^* + S6 + S6^*). \quad (3.57)$$

The classical limit of the $|\alpha|^9$, $|\alpha|^7$, and $|\alpha|^5$ terms can be found with the aid of Eqs. (B11) and (B14). Keeping only the first term of σ [see Eq. (B12)], we have that

$$\begin{aligned} \lim_{CLCS} \lambda^2 \langle \hat{x} \rangle^{(2)} &= \frac{A^5 \lambda^2}{16\omega_0^4 m^2} \left[\frac{23}{4} \cos(Wt) - 6 \cos(3Wt) + \frac{1}{4} \cos(5Wt) \right] + \frac{93A^7 \lambda^3 t}{64m^3 \omega_0^5} \sin(Wt) \\ &\quad - \frac{45A^7 \lambda^3 t}{64m^3 \omega_0^5} \sin(3Wt) - \frac{225A^9 \lambda^4 t^2}{128m^4 \omega_0^6} \cos(Wt) + O(\lambda^4). \end{aligned} \quad (3.58)$$

Comparing Eqs. (3.56) and (3.58) with Eq. (3.52), we see that we can account for the secular terms which arise from the classical limit of the BD method. *In addition, if Eq. (3.51) is used to write the results of Eqs. (3.50), (3.56), and (3.58) in terms of ω , and the trigonometric functions involving $(\omega - W)$ are replaced by the first few terms of their Taylor series expansions, we obtain the Poincaré–Lindstedt perturbation expansion of Eqs. (2.8) and (2.9).*

In summary, the application of the CLCS to the quantum perturbation expansion yielded by Method 1 produces a classical expansion with secular terms. However, if the Poincaré–Lindstedt perturbation expansion to the initial value problem of Eqs. (2.6) and (2.7) is written in terms of the frequency expansion obtained from Method 1 and then expanded, an identical expansion with secular terms is obtained. *Conversely, the classical expansion yielded by Method 1, complete with secular terms, can be transformed into the Poincaré–Lindstedt perturbation expansion.*

D. Classical limit of Method 2 (BD)

This proceeds in a manner similar to that of Method 1 above. In order to avoid confusion with the constant A of Method 1, we denote the CLCS here as $\hbar \rightarrow 0$, $|\alpha| \rightarrow \infty$, with $\hbar |\alpha|^2 = \mathcal{A}^2 m \omega_0 / 2$. The result is

$$\begin{aligned} \langle \Phi(x, t) | \hat{x} | \Phi(x, t) \rangle_{CLCS} &= \mathcal{A} \cos(\mathcal{W}t) + \frac{\mathcal{A}^3 \lambda}{8m\omega_0^2} [\cos(3\mathcal{W}t) - 6 \cos(\mathcal{W}t)] \\ &\quad + \frac{\mathcal{A}^5 \lambda^2}{128\omega_0^4 m^2} [303 \cos(\mathcal{W}t) - 78 \cos(3\mathcal{W}t) + 2 \cos(5\mathcal{W}t)] + \dots, \end{aligned} \quad (3.59)$$

with

$$\mathcal{W} = \omega_0 + \frac{3\mathcal{A}^2 \lambda}{2m\omega_0} - \frac{51\mathcal{A}^4}{16m^2 \omega_0^3} \lambda^2 + \frac{375\mathcal{A}^6}{32m^3 \omega_0^5} \lambda^3 + \dots \quad (3.60)$$

In order to compare these results with the classical Poincaré–Lindstedt results of Eqs. (2.8) and (2.9), we need to invert the series

$$\langle \Phi(x, 0) | \hat{x} | \Phi(x, 0) \rangle = A = \mathcal{A} - \frac{5\mathcal{A}^3}{8m\omega_0^2} \lambda + \frac{227}{128} \frac{\mathcal{A}^5}{m^2 \omega_0^4} \lambda^2 + \dots, \quad (3.61)$$

to obtain

$$\mathcal{A} = A + \frac{5}{8} \frac{A^3}{m\omega_0^2} \lambda - \frac{77}{128} \frac{A^5}{m^2\omega_0^4} \lambda^2 + \dots \quad (3.62)$$

When this expansion for \mathcal{A} is substituted into Eqs. (3.59) and (3.60), then the classical Poincaré–Lindstedt expansions of Eqs. (2.8) and (2.9) are obtained.

In addition we have

$$\begin{aligned} \langle \Psi(x, t) | \hat{p} | \Psi(x, t) \rangle_{CLCS} = & -\mathcal{A} m \omega_0 \sin(\mathcal{W}t) - \frac{\mathcal{A}^3 \lambda}{8 \omega_0} [3 \sin(3 \mathcal{W}t) + 6 \sin(\mathcal{W}t)] \\ & + \frac{\mathcal{A}^5 \lambda^2}{64 m \omega_0^3} \left[-5 \sin(5 \mathcal{W}t) + 81 \sin(3 \mathcal{W}t) + \frac{249}{2} \sin(\mathcal{W}t) \right] + \dots, \end{aligned} \quad (3.63)$$

with \mathcal{W} as given in Eq. (3.60). Once the substitution of Eq. (3.62) is made, then the classical Poincaré–Lindstedt expansion for $p(t)$ of Eq. (2.10) is obtained.

In summary, the CLCS applied to Method 2 also yields a Poincaré–Lindstedt perturbation expansion for a classical periodic orbit. However the amplitude \mathcal{A} of this orbit is given by Eq. (3.62) and not simply A . This is in analogy to the situation for classical orbits shown in Section II.

IV. THE CONNECTION BETWEEN THE $N\hbar$ AND THE $|\alpha|^2\hbar$ CLASSICAL LIMITS FOR THE HARMONIC OSCILLATOR PROBLEM

The connection between the $N\hbar$ and the $|\alpha|^2\hbar$ classical limits (for time independent and time dependent perturbation theories, respectively) is not obvious apart from the common mathematical operation of letting $\hbar \rightarrow 0$. This section will provide some insight by investigating the classical limit of the quantum probability density for the harmonic oscillator problem.

A. The classical probability density

Here we assume the special case of a bounded periodic orbit in one spatial dimension in a potential well $V(x)$ with turning points at x_1 and x_2 . Since the classical probability density is inversely proportional to the the velocity ($v(x)$),

$$P_{cl}(x) = N \frac{1}{\sqrt{E - V(x)}}, \quad (4.1)$$

where N is determined by the normalization condition

$$\int_{x_1}^{x_2} P_{cl}(x) dx = 1. \quad (4.2)$$

For the harmonic oscillator,

$$V(x) = \frac{m\omega_0^2}{2} x^2, \quad (4.3)$$

the turning points are and $x_1 = -A$ and $x_2 = A$, where

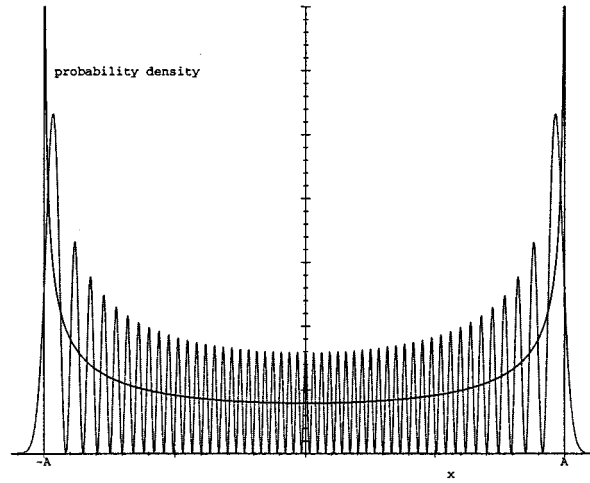


FIG. 1. The classical ($P_{cl}(x)$) and quantum ($|\phi_n^{(0)}(x)|^2, n=50$) probability densities for the harmonic oscillator.

$$A = \sqrt{\frac{2E}{m\omega_0^2}} = \sqrt{\frac{2J}{m\omega_0}}, \quad (4.4)$$

and J is the classical action of the orbit. Thus,

$$P_{cl}(x) = \begin{cases} \frac{1}{\pi\sqrt{A^2-x^2}}, & \text{for } |x| < A, \\ 0, & \text{for } |x| > A. \end{cases} \quad (4.5)$$

The classical probability density along with the corresponding quantum probability density is depicted in Fig. 1.

B. The probability density of the harmonic oscillator coherent state and its classical limit

Consider the probability distribution for the harmonic oscillator coherent state and its classical limit given in Eq. (3.12). In order to compare this result with the probability density for an ensemble of classical orbits given in Eq. (4.5), we can take a time average over one period of oscillation,⁴² $T = 2\pi/\omega_0$:

$$\lim_{CLCS} \frac{1}{T} \int_0^T |\Psi^{(0)}(x,t)|^2 dt = \frac{1}{T} \int_0^T \delta[x - A \cos(\omega_0 t + \varphi)] dt. \quad (4.6)$$

Using the fact that [Ref. 8, p. 1471, Eq. (21)]

$$\delta[g(t)] = \sum_j \frac{\delta(t-t_j)}{|g'(t_j)|}, \quad (4.7)$$

where the t_j are the simple zeroes of $g(t)$, it can be shown that the right hand side of Eq. (4.6) is equal to the classical probability density in Eq. (4.5).

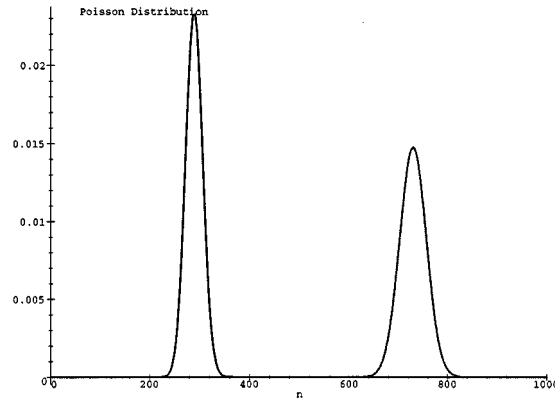


FIG. 2. The Poisson distribution $e^{-|\alpha|^2}|\alpha|^{2n}/n!$. The first peak corresponds to $|\alpha|=17$ and the second to $|\alpha|=27$.

Now consider the coherent state written in terms of the harmonic oscillator stationary state basis functions:

$$\Psi^{(0)}(x,t) = e^{-|\alpha|^2/2} \sum_{n=0}^{\infty} \frac{\alpha^n}{\sqrt{n!}} \exp\left[-it\omega_0\left(n + \frac{1}{2}\right)\right] \phi_n^{(0)}(x). \quad (4.8)$$

The time average of the magnitude of the above wavefunction is

$$\frac{1}{T} \int_0^T |\Psi^{(0)}(x,t)|^2 dt = e^{-|\alpha|^2} \sum_{n=0}^{\infty} \frac{|\alpha|^{2n}}{n!} |\phi_n^{(0)}|^2. \quad (4.9)$$

The coefficients of this sum constitute a Poisson density function,

$$\frac{e^{-|\alpha|^2} |\alpha|^{2n}}{n!}, \quad (4.10)$$

which is plotted in Fig. 2. If we assume for the moment that n is a continuous variable, (say x), we can write the Poisson density function in terms of the gamma function,

$$f(x) = \frac{e^{-|\alpha|^2} |\alpha|^{2x}}{\Gamma(x+1)}. \quad (4.11)$$

The derivative of $f(x)$ is given by

$$f'(x) = \frac{e^{-|\alpha|^2} |\alpha|^{2x} [\ln|\alpha|^2 - \psi(x+1)]}{\Gamma(x+1)}, \quad (4.12)$$

where $\psi(\cdot)$ is the digamma (or psi) function [see Abramowitz and Stegun,⁴³ p. 258, Eq. (6.3.1)]. From Abramowitz and Stegun,⁴³ p. 259, Eq. (6.3.18),

$$\psi(x+1) \sim \ln(x+1) - \frac{1}{(2x+2)} + \cdots, \quad x \rightarrow \infty, \quad (4.13)$$

so that there is a critical point at $x \approx |\alpha|^2 - 1$, for large x (and hence for large $|\alpha|$). This means that the maximum of the Poisson distribution is approximately located at $n \approx |\alpha|^2$ for large $|\alpha|$. The fact that the dominant contribution in the sum of harmonic oscillator wavefunctions is due to those functions with quantum numbers in the neighborhood of $n \approx |\alpha|^2$ was noted by Schrödinger in his paper which introduced the harmonic oscillator coherent states.^{6,7} Let N denote the value of n with the maximum contribution to the sum in Eq. (4.9) (i.e., $N \approx |\alpha|^2$). Note that the maximum does *not* become sharper and higher as $|\alpha|$ increases. From Abramowitz and Stegun,⁴³ p. 929 the variance of the Poisson distribution is $|\alpha|^2$ so that the distribution spreads out as $|\alpha|$ increases (see Fig. 2). This means that the classical limit of coherent states does not just select a single wavefunction at $n \approx |\alpha|^2$. Instead, an increasing number of wavefunctions are included in the classical limit. This supports Ballentine's statement⁴⁴ that the classical limit of a quantum state is an ensemble of classical orbits, not a single classical orbit.

We have already shown, using the x -representation of the probability density that Eq. (4.9) goes to the classical probability density in the CLCS [see Eqs. (4.6) and (4.7)]. The proof of this fact using the representation in terms of the harmonic oscillator stationary states [i.e., the right hand side of Eq. (4.9)], is less elegant but it does however provide some insight into the interplay between the CLCS [see Eq. (3.11)] and the $\hbar \rightarrow 0$, $n \rightarrow \infty$, $n\hbar = J$ limit for stationary states.

The basic idea (inspired by Liboff,⁴⁵ p. 55) is to use the change of variables

$$z = \frac{n - |\alpha|^2}{|\alpha|} \quad (4.14)$$

to transform the sum weighted by a discrete Poisson distribution to an integral weighted by a continuous Gaussian distribution. Using Stirling's formula [see Abramowitz and Stegun,⁴³ p. 257, Eq. (6.1.37)], one can show that

$$\frac{e^{-|\alpha|^2} |\alpha|^{2n+1}}{n!} \sim \frac{1}{\sqrt{2\pi}} \exp\left(-\frac{z^2}{2}\right), \quad |\alpha| \rightarrow \infty. \quad (4.15)$$

Note that since $n = N(1 + z/|\alpha|)$, the WKB approximation⁴⁶ for $|\phi_n^{(0)}(x)|^2$ is valid in the CLCS. It can be shown that the WKB approximation for $|\phi_n^{(0)}(x)|^2$ goes to zero in the CLCS for $|x| > A$, where A is given in Eq. (4.4). For $-A < x < A$,

$$|\phi_{nWKB}^{(0)}(x)|^2 = \frac{m\omega_0}{\pi\sqrt{-Q(x)}} \left\{ 1 + \sin\left[\frac{2}{\hbar} \int_{-A}^x \sqrt{-Q(y)} dy\right] \right\}, \quad (4.16)$$

where $Q(x) = m^2 \omega_0^2 x^2 - 2mE$. Letting $J_n = n\hbar$ and $J_N = N\hbar$,

$$\frac{1}{\hbar} = \frac{n}{J_n} = \frac{|\alpha|z + |\alpha|^2}{J_n} \sim \frac{|\alpha|z + |\alpha|^2}{J_N}, \quad |\alpha| \rightarrow \infty, \quad (4.17)$$

so that

$$e^{-|\alpha|^2} \sum_{n=0}^{\infty} \frac{|\alpha|^{2n}}{n!} |\phi_n^{(0)}(x)|^2 \sim \frac{1}{\sqrt{2\pi^3(A^2 - x^2)}} \int_{-\infty}^{\infty} e^{-z^2/2} \times \left\{ 1 + \sin\left[\left(\frac{2|\alpha|z}{J_N} + \frac{|\alpha|^2}{J_N}\right) \int_{-A}^x \sqrt{-Q(y)} dy\right] \right\} dz. \quad (4.18)$$

Since the second part of the integral vanishes as $|\alpha| \rightarrow \infty$, we have the required result. See the thesis of McRae²⁰ for more details of this proof.

V. CONCLUSIONS

A major goal of this paper has been to point out several aspects of the method of BD⁵ which have not previously appeared in the literature. It is misleading to state that the BD method can be easily extended to higher orders or that taking the classical limit of the results of this method is an efficient approach to performing classical perturbation theory. As we have seen, in general, the second order calculations involve infinite summations for which a closed form cannot be found. If the initial condition is chosen to be a harmonic oscillator coherent state (Method 1), secular terms emerge in the classical limit. Knowing the classical frequency (ω), these results can be rewritten in terms of ω to remove these secular terms and obtain the classical Poincaré–Lindstedt expansion. If the initial condition is chosen to be a perturbed coherent state [see Eq. (3.43)], as has been done in the literature, then the resulting solution must be rearranged in order to agree with the classical solution for higher orders in the perturbation parameter.

We have been able to pinpoint the location of secular terms which cause problems in the classical limit when the initial conditions of Method 1 are assumed. In S3, the terms of order α^4 and α^5 (which would lead to secular terms in the classical limit) cancel each other out in the expression $\langle \phi_m^{(0)} | \hat{a} | \phi_n^{(1)} \rangle + \langle \phi_m^{(1)} | \hat{a} | \phi_n^{(0)} \rangle$. Similarly in S5, terms of order α^6 to α^9 disappear through cancellation in the expression $\langle \phi_m^{(0)} | \hat{a} | \phi_n^{(2)} \rangle + \langle \phi_m^{(1)} | \hat{a} | \phi_n^{(1)} \rangle + \langle \phi_m^{(2)} | \hat{a} | \phi_n^{(0)} \rangle$. These fortuitous cancellations do not occur in the expression $C_n^{(0)} C_m^{*(1)} + C_n^{(1)} C_m^{*(0)}$ in S2 and S6, or in the expression $C_n^{(2)} C_m^{*(0)} + C_n^{(1)} C_m^{*(1)} + C_n^{(0)} C_m^{*(2)}$ in S4, causing secular terms to emerge in the classical limit. Admittedly, a deeper reason for this appearance of secular terms is not known at this time. In addition, there remains the question of whether secular terms will emerge at higher orders from the second choice of initial conditions. Clearly further work is needed to understand these problems completely. We hope that our study would inspire further investigations.

The method of Bhattacharyya^{32,33} has also been investigated²⁰ using the initial conditions of a HOCS. It is found to yield the same results as BD Method 1. As such, Bhattacharyya's method will encounter the same problem of secular terms emerging in the classical limit for this initial condition.

Obtaining classical Poincaré–Lindstedt perturbation expansions from a classical limit of coherent states is not unexpected. It turns out that the classical limit of coherent states given in Eq. (3.11) is also valid for solutions of the time development of a harmonic oscillator coherent state in an anharmonic potential. Several authors^{47–51} have considered classical limits of coherent state time evolution. In particular, Hagedorn⁴⁹ rigorously proved a result originally introduced by Heller.⁵² Heller calculated the time evolution of certain Gaussian wave packets semi-classically. Hagedorn rigorously showed that the quantum evolution of these wave packets approaches the classical solution asymptotically as $\hbar \rightarrow 0$. At this point, it is appropriate to mention that Combescure⁵³ has extended Hagedorn's results to the case of explicitly time dependent periodic Hamiltonians where the classical equations of motion possess periodic orbits.

In Section IV, we have shown the connection between two types of classical limit which share the common mathematical operation of letting $\hbar \rightarrow 0$. The classical limit for coherent states also involves the $n\hbar = J$ limit for energy eigenstates. In the harmonic oscillator (and perturbed anharmonic oscillator), the connection between the two limits implies that an increasing number of eigenstates are included as $\hbar \rightarrow 0$ in order to produce a delta function distribution which is centered on the classical periodic orbit.

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APPENDIX A: CLASSICAL LIMIT OF RSPT

It has been shown that a classical limit of the quantum mechanical Rayleigh–Schrödinger perturbation series (see for example the review article of Hirschfelder *et al.*⁴¹) for the energy eigenvalues can be taken to yield the classical canonical (i.e., action preserving) perturbation series. Turchetti³ was the first to study the classical limit of the Rayleigh–Schrödinger perturbation series for one dimensional anharmonic oscillators. For more on the results of this section see the paper of McRae and Vrscaj¹ and references therein.

Quantum mechanically, the eigenvalue problem to be solved is

$$[\hat{H}^{(0)} + \lambda \hat{V}] \phi_n(x) = E_n \phi_n(x), \quad (\text{A1})$$

where the solutions of the unperturbed eigenvalue problem,

$$\hat{H}^{(0)} \phi_n^{(0)}(x) = E_n^{(0)} \phi_n^{(0)}(x), \quad (\text{A2})$$

are known. In the above equations, $\hat{H}^{(0)}$ denotes the unperturbed quantum Hamiltonian, λ is the perturbation parameter, \hat{V} is the perturbing potential, $\phi_n(x)$, $\phi_n^{(0)}(x)$, E_n , and $E_n^{(0)}$ are the eigenfunctions and the energy eigenvalues of the perturbed and unperturbed systems, respectively. Using Rayleigh–Schrödinger perturbation theory, a perturbation series for the energy,

$$E_n(\hbar) = \sum_{j=0}^{\infty} E_n^{(j)}(\hbar) \lambda^j, \quad (\text{A3})$$

can be calculated.

In the corresponding classical situation, consider a Hamiltonian of the form

$$H(x, p) = H^{(0)}(x, p) + \lambda V(x), \quad (\text{A4})$$

where $H^{(0)}(x, p)$ is the Hamiltonian of the unperturbed classical system, λ is the perturbation parameter, and $V(x)$ is the perturbing potential. One can use Poincaré–von Zeipel perturbation theory to find a perturbation expansion for the classical energy in terms of the action variable J :

$$E(J) = \sum_{j=0}^{\infty} E^{(j)}(J) \lambda^j. \quad (\text{A5})$$

It is not immediately obvious which classical energy out of an infinite continuum of possible energies is being calculated in the perturbation series of Eq. (A5). It turns out to be the energy of the periodic orbit in phase space that possesses the same action J as the unperturbed system. This is due to the fact that classical canonical perturbation theory preserves the action.

The appropriate classical limit for Turchetti's result is $\hbar \rightarrow 0$, $n \rightarrow \infty$, with $n\hbar = J$. In this limit, the quantum perturbation series for E_n goes to the classical perturbation series for E .

Graffi and Paul⁴ have rigorously proved the validity of the $n\hbar$ classical limit for the N dimensional harmonic oscillator with nonresonant frequencies and an entire holomorphic perturb-

ing potential. Alvarez, Graffi and Silverstone⁵⁴ have shown that the Rayleigh–Schrödinger perturbation series for the energy can be rearranged to give the classical series plus convergent subseries that give corrections in powers of \hbar , through investigations of the quartic⁵⁴ and cubic⁵⁵ one dimensional anharmonic oscillators. McRae and Vrscaj^{56,1} introduced a method of calculating the classical energy series of Eq. (A5) analogous to the quantum Hellmann–Feynman method, which is easier to calculate to large order than the Poincaré–von Zeipel method. The classical limit of perturbation series for radial hydrogenic problems was also investigated. Finally, it is important to mention another method of classical perturbation theory, the Birkhoff,⁵⁷ Gustavson⁵⁸ normal form perturbation theory and its quantum analogue.^{59–64}

APPENDIX B: CLASSICAL LIMIT RESULTS FOR THE BD METHOD

This appendix contains several results which are useful for calculating classical limits of expressions from the BD method. If we only keep terms to first order in λ , the BD solutions are made up of summations of the form

$$e^{-|\alpha|^2} \sum_{n=0}^{\infty} \frac{|\alpha|^{2n}}{n!} \exp[a + b\hbar\lambda(n+c)] \quad (\text{B1})$$

(where a , b and c are constants), for which a closed form can be found and the classical limit taken. If higher order terms in λ are retained, then the exponentials will contain terms of order n^2 and higher and a closed form for the summations can no longer be found. In this case, the results of this appendix are required in order to obtain the classical limit. In the literature,^{5,9–17} only first order perturbative solutions have been given so that the details of the complications which occur for taking the classical limit of higher order terms have not been published before.

The following result may be proved by induction using properties of Stirling numbers of the second kind which can be found in Abramowitz and Stegun⁴³ on p. 824,

$$\begin{aligned} e^{-|\alpha|^2} \sum_{n=0}^{\infty} \exp\left[\frac{it}{\hbar}(E_{n+j}-E_{n+k})\right] \frac{|\alpha|^{2n}}{n!} n^p \\ = e^{-|\alpha|^2} \sum_{l=0}^{p-1} \mathcal{S}_p^{(p-l)} \sum_{n=0}^{\infty} \exp\left[\frac{it}{\hbar}(E_{n+j+p-l}-E_{n+k+p-l})\right] \frac{|\alpha|^{2(n+p-l)}}{n!}, \end{aligned} \quad (\text{B2})$$

for $p = 1, 2, \dots$, where $\mathcal{S}_n^{(m)}$ are Stirling numbers of the second kind. Note that for the special case of $j=k$ we have

$$e^{-|\alpha|^2} \sum_{n=0}^{\infty} \frac{|\alpha|^{2n}}{n!} n^p = \sum_{l=0}^{p-1} \mathcal{S}_p^{(p-l)} |\alpha|^{2(p-l)}, \quad \text{for } p \geq 1. \quad (\text{B3})$$

The following result was first proved by Benoit.¹⁸

$$L = \lim_{CLCS} e^{-|\alpha|^2} \sum_{n=0}^{\infty} \frac{|\alpha|^{2n}}{n!} \exp\left[\sum_{j=0}^{\infty} \hbar^j \sum_{k=0}^j a_{j,k} n^k\right] = \exp\left[\sum_{k=0}^{\infty} a_{k,k} \gamma^k\right], \quad (\text{B4})$$

where γ and $CLCS$ are defined in Eq. (3.11). The above limit may be proved by expanding the exponential in the left hand side of Eq. (B4) in a Taylor series, rearranging so that all of the \hbar terms are collected together, and then using the result which follows to take the classical limit. From Eq. (B3),

$$e^{-|\alpha|^2} \sum_{n=0}^{\infty} \frac{|\alpha|^{2n}}{n!} \hbar^j n^k = \sum_{i=0}^{k-1} \mathcal{A}_k^{(k-i)} |\alpha|^{2(k-i)} \hbar^j, \quad k \geq 1, \quad (\text{B5})$$

so that

$$\lim_{CLCS} e^{-|\alpha|^2} \sum_{n=0}^{\infty} \frac{|\alpha|^{2n}}{n!} \hbar^j n^k = \begin{cases} \gamma^j, & \text{if } k=j, \\ 0, & \text{if } j>k, \\ \infty, & \text{if } j<k. \end{cases} \quad (\text{B6})$$

As a particular case, consider the classical limit of

$$S = e^{-|\alpha|^2} \sum_{n=0}^{\infty} \exp \left[\frac{it}{\hbar} (E_{n+j} - E_{n+k}) \right] \frac{|\alpha|^{2n}}{n!}. \quad (\text{B7})$$

Using the series expansion of Eq. (3.17) and Eqs. (3.19)–(3.22), for the quartic anharmonic oscillator, we have

$$\lim_{CLCS} e^{-|\alpha|^2} \sum_{n=0}^{\infty} \exp \left[\frac{it}{\hbar} (E_{n+j} - E_{n+k}) \right] \frac{|\alpha|^{2n}}{n!} = \exp[it(j-k)W], \quad (\text{B8})$$

where

$$\begin{aligned} W &= \omega_0 + \frac{3\gamma}{m^2 \omega_0^2} \lambda - \frac{51}{4} \frac{\gamma^2}{m^4 \omega_0^5} \lambda^2 + \frac{375}{4} \frac{\gamma^3}{m^6 \omega_0^8} \lambda^3 + O(\lambda^4) \\ &= \omega_0 + \frac{3A^2}{2m\omega_0} \lambda - \frac{51}{16} \frac{A^4}{m^2 \omega_0^3} \lambda^2 + \frac{375}{32} \frac{A^6}{m^3 \omega_0^5} \lambda^3 + O(\lambda^4). \end{aligned} \quad (\text{B9})$$

Note that in deriving Eq. (B4) we expanded the exponential. This means that the resulting classical limit is valid only for finite times.

Using similar techniques, it may be shown that

$$\begin{aligned} \lim_{CLCS} |\alpha|^2 e^{-|\alpha|^2} \sum_{n=0}^{\infty} \frac{|\alpha|^{2n}}{n!} \left\{ \exp \left[\sum_{j=0}^{\infty} \hbar^j \sum_{k=0}^j a_{j,k} n^k \right] - \exp \left[\sum_{j=0}^{\infty} \hbar^j \sum_{k=0}^j b_{j,k} n^k \right] \right\} \\ = \exp \left[\sum_{j=0}^{\infty} a_{jj} \gamma^j \right] \sum_{k=1}^{\infty} (a_{k,k-1} - b_{k,k-1}) \gamma^k, \end{aligned} \quad (\text{B10})$$

when $a_{jj} = b_{jj}$ for $j = 0, \dots, \infty$. Applying the above result to the situation which arises in the BD calculations,

$$\lim_{CLCS} |\alpha|^2 e^{-|\alpha|^2} [T_{j,k} - T_{J,K}] = \exp[it(j-k)W] it(j^2 - k^2 - J^2 + K^2) \sigma, \quad (\text{B11})$$

when $j - k = J - K$, where W is given in Eq. (B9) and

$$\sigma = \frac{3A^2 \lambda}{4m\omega_0} - \frac{51A^4 \lambda^2}{16m^2 \omega_0^3} + \frac{1125A^6 \lambda^3}{64m^3 \omega_0^5} + \dots \quad (\text{B12})$$

The final result is

$$\begin{aligned}
& \lim_{CLCS} |\alpha|^4 e^{-|\alpha|^2} \sum_{n=0}^{\infty} \frac{|\alpha|^{2n}}{n!} \left\{ \exp \left[\sum_{j=0}^{\infty} \hbar^j \sum_{k=0}^j a_{jk} n^k \right] + \exp \left[\sum_{j=0}^{\infty} \hbar^j \sum_{k=0}^j b_{jk} n^k \right] \right. \\
& \quad \left. - 2 \exp \left[\sum_{j=0}^{\infty} \hbar^j \sum_{k=0}^j d_{jk} n^k \right] \right\} \\
& = \exp \left[\sum_{j=0}^{\infty} a_{jj} \gamma^j \right] \sum_{k=2}^{\infty} \gamma^k \left\{ -(a_{k,k-2} + b_{k,k-2} - 2d_{k,k-2}) \right. \\
& \quad \left. + \frac{1}{2} \sum_{i=1}^{k-1} (a_{i,i-1} a_{k-i,k-i-1} + b_{i,i-1} b_{k-i,k-i-1} - 2d_{i,i-1} d_{k-i,k-i-1}) \right\}, \quad (B13)
\end{aligned}$$

when $a_{jj}=b_{jj}=d_{jj}$ and $a_{j,j-1}+b_{j,j-1}-2d_{j,j-1}=0$. This enables us to calculate the classical limit of terms such as the $|\alpha|^9$ term in Eq. (3.40):

$$\begin{aligned}
& \lim_{CLCS} |\alpha|^4 e^{-|\alpha|^2} [T_{j,k} + T_{J,K} - 2T_{\mathcal{J},\mathcal{K}}] \\
& = \exp[it(j-k)W] \left\{ \frac{A^4 \lambda^2}{4m^2 \omega_0^2} \left[\frac{-9t^2}{8} (j-k)^2 [(j+k)^2 + (J+K)^2 - 2(\mathcal{J}+\mathcal{K})^2] \right. \right. \\
& \quad \left. \left. + \frac{it}{\omega_0} [j^3 - k^3 + J^3 - K^3 - 2(\mathcal{J}^3 - \mathcal{K}^3)] + O(\lambda^3) \right] \right\}, \quad (B14)
\end{aligned}$$

when $j-k=J-K=\mathcal{J}-\mathcal{K}$ and $j^2-k^2+J^2-K^2-2(\mathcal{J}^2-\mathcal{K}^2)=0$.

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