Canonical perturbation expansions to large order from classical hypervirial and Hellmann–Feynman theorems

Cite as: Journal of Mathematical Physics **33**, 3004 (1992); https://doi.org/10.1063/1.529521
Submitted: 17 May 1991 . Accepted: 15 April 1992 . Published Online: 04 June 1998

S. M. McRae, and E. R. Vrscay

Canonical perturbation expansions to large order from classical hypervirial and Hellmann–Feynman theorems

S. M. McRae and E. R. Vrscay
Department of Applied Mathematics, Faculty of Mathematics, University of Waterloo, Waterloo, Ontario N2L 3G1, Canada

(Received 17 May 1991; accepted for publication 15 April 1992)

The classical hypervirial and Hellmann–Feynman theorems are used to formulate a "perturbation theory without Fourier series" that can be used to generate canonical series expansions for the energies of perturbed periodic orbits for separable classical Hamiltonians. As in the case where these theorems are used to generate quantum mechanical Rayleigh–Schrödinger perturbation series, the method is very efficient and may be used to generate expansions to large order either numerically or in algebraic form. Here, the method is applied to one-dimensional anharmonic oscillators and radial Kepler problems. In all cases, the classical series for energies and expectation values are seen to correspond to the expansions associated with their quantum mechanical counterparts through an appropriate action preserving classical limit as discussed by Turchetti, Graffi, and Paul. This "action fixing" is inherent in the classical Hellmann–Feynman theorem applied to periodic orbits.

I. INTRODUCTION

In this paper we describe a method of generating perturbation expansions for the energies of (multiply) periodic orbits of simple perturbed, separable, classical Hamiltonians. The expansions afforded by this method are precisely those given by traditional canonical perturbation theory, often referred to as the Poincaré–von Zeipel method[1–3] or the Birkhoff expansion.[4] The method described here employs the classical versions of two well-known and useful quantum mechanical theorems, namely, the hypervirial (HV)[5] and Hellmann–Feynman (HF)[6] theorems. The use of the quantum mechanical HV and HF theorems to provide perturbation expansions is well known.[7,8] The classical versions of these theorems are also well known[9,10] but have not, to our knowledge, been exploited in such a way. Our approach, which may be viewed as a classical analog of the quantum HVHF perturbation method, utilizes the recursion relations between time averages and the energy of a classical periodic orbit, as provided by the classical HV theorem. Applicable only to separable problems, it provides a very efficient algorithm for the generation of classical perturbation expansions to large order, replacing the formal manipulation of Fourier series expansions with recursion relations.

The fact that the classical HVHF method yields the Birkhoff expansion for the energy is due to the connection between the classical Hellman–Feynman theorem and the principle of least action. As such, the expansions are consistent with the canonical perturbation series obtained from other methods, including Birkhoff–Gustavson normal forms[11,12] and Lie theory.[13] As well, they also correspond to the classical series obtained from traditional Rayleigh–Schrödinger (RS) perturbation expansions (for nonresonant oscillators) when an appropriate classical limit is taken while keeping the value of the classical action fixed.[14–17]

It is beyond the scope of this paper to discuss the many attempts to construct accurate semiclassical and quantum perturbation expansions for the more difficult case of nonintegrable Hamiltonian systems, e.g., the Henon–Heiles system. However, it would be helpful to mention some works, namely, (i) that of Swimm and Delos,[18] who used the Birkhoff–Gustavson method of normal forms (BGNF) to perform semiclassical quantization on a nonintegrable system, and (ii) further development by Reinhardt and co-workers.[19] Although these semiclassical calculations show good agreement with the "exact" quantum results, there is still no general method for obtaining the exact quantum series from the classical BGNF series for the nonintegrable case. Robnik[20] and Wood and Ali[21] made attempts in this direction. Ali[22] and Eckhardt[23] reformulated the BGNF in terms of Lie algebras to develop an analogous quantum perturbation theory, the quantum normal form (QNF). The QNF was shown to be equivalent to the usual Rayleigh–Schrödinger perturbation theory and that the BGNF can be obtained from QNF in a classical limit. These methods have been applied to several examples.[24]

The layout of the paper is as follows. In Sec. II, the classical and quantum mechanical settings are outlined, along with their respective perturbation theories. In Sec. III we review the quantum mechanical HV and HF theorems, as well as the associated "perturbation theory without wave functions." Section IV is devoted to the classical HV and HF theorems and their proofs and de-

 0022-2488/92/093004-21$03.00

scribes the new perturbation procedure. The reader interested in first seeing the method without the background should proceed directly to this section. Some illustrative examples are presented in Sec. V, including one-dimensional anharmonic oscillators and radial hydrogenic problems. In the appropriate "canonical" classical limit, the quantum mechanical series for the eigenvalues become the respective classical series. This classical limit is also observed for the perturbation expansions associated with the expectation values, e.g., $\langle x^k \rangle$. This feature may be viewed as a consequence of the classical limit of the Wigner function associated with the mechanical system. Our results show that the classical limit for RSPT/expectation values also exists for perturbed hydrogenic problems: these classical series are relevant to the study of perturbed Kepler problems.

Finally, we mention that the algebraic computations reported in this paper were performed using the symbolic computation language MAPLE.[25]

II. THE CLASSICAL AND QUANTUM SETTINGS

In this section we outline the classical and corresponding quantum mechanical systems to be studied, with a review of the relevant ideas behind classical dynamics in phase space. In no way is the discussion intended to be complete: the material is covered extensively in standard books on mechanics[1-3,26] and dynamical systems theory.[27,28]

A. The classical case

In the framework of Hamiltonian mechanics, we consider the motion of a particle of mass m in $\mathbf{R}^D$, $D=1,2,...$, under the influence of a (smooth) scalar potential, $V:\mathbf{R}^D \to \mathbf{R}$, $V \in C^r(S_0)$, $r \geqslant 2$, where $S_0 \subset \mathbf{R}^D$ is open and bounded. Let $\mathbf{q}(t)=(q_1(t),...,q_D(t))$ denote the position of the mass at time t. The classical Hamiltonian for this system is given by

$$H(\mathbf{p},\mathbf{q})=\frac{p^2}{2m}+V(\mathbf{q})=\frac{1}{2m}\sum_{i=1}^{D} p_i^2+V(q_1,...,q_D), \tag{2.1}$$

where the p_i, $i=1,2,...,D$, denote the canonical momenta conjugate to the coordinates q_i. If $(\mathbf{p}(0),\mathbf{q}(0))=(\mathbf{p}_0,\mathbf{q}_0)$, then a complete description of the motion is provided by the trajectory of $(\mathbf{p}(t),\mathbf{q}(t))$ in phase space $\mathbf{R}^{2D}$ as defined by Hamilton's equations,

$$\dot{q}_i=\frac{\partial H}{\partial p_i}, \quad \dot{p}_i=-\frac{\partial H}{\partial q_i}, \quad i=1,2,...,D, \tag{2.2}$$

with the above initial conditions. This set of $2D$ first-order differential equations defines a dynamical system[27] in $\mathbf{R}^{2D}$. The points $(\mathbf{p},\mathbf{q})=(0,\bar{\mathbf{q}})$, where $\bar{\mathbf{q}}$ is a critical point of $V(\mathbf{q})$, are equilibrium points. By a theorem of Lagrange,[27] if $\bar{\mathbf{q}}$ is a local minimum of V, then $(0,\bar{\mathbf{q}})$ is Lyapunov stable. If $\bar{\mathbf{q}}$ is a local maximum or saddle point, then $(0,\bar{\mathbf{q}})$ is unstable.

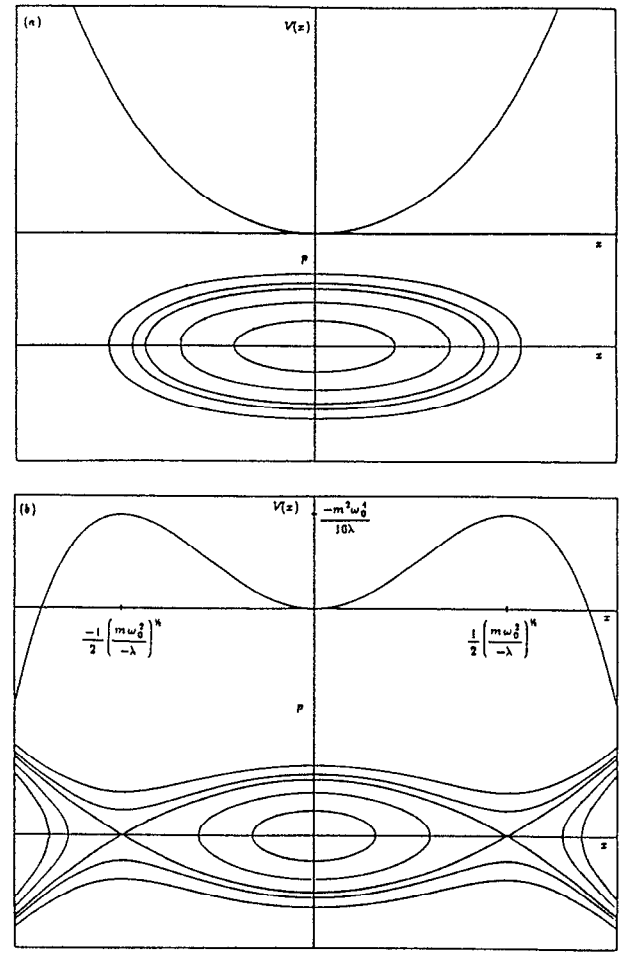

FIG. 1. Typical plots of the one-dimensional potential energy function for the classical quartic anharmonic oscillator [$M=4$ in Eq. (2.12)], $V(x)=\frac{1}{2}m\omega_0^2x^2+\lambda x^4$ and corresponding phase portraits below: (a) $\lambda > 0$: all orbits are bounded and periodic; (b) $\lambda < 0$: only orbits with energies $\bar{E} < -m^2\omega_0^4/16\lambda$ are bounded and periodic.

Of principal concern are the bounded periodic orbits that correspond to oscillations about a local minimum $\bar{\mathbf{q}}$ of the potential $V(\mathbf{q})$. Sketches of typical situations for a one-dimensional potential are shown in Fig. 1. A variety of perturbation methods have been developed to study the behavior of such orbits under perturbations of the potential. Our treatment is restricted to time-independent Hamiltonians of the form in (2.1) that are completely separable (hence integrable), i.e., reducible to a set of D one-dimensional problems, each of which is periodic. This may be expressed in terms of the Hamilton–Jacobi (HJ) equation associated with Eq. (2.1):[1-3]

$$H\left(\frac{\partial W}{\partial \mathbf{q}},\mathbf{q}\right)=\bar{E}. \tag{2.3}$$

(Note: In this paper, classical energy functions will be "barred" in order to distinguish them from quantum mechanical energies.) For separable Hamiltonians H, the characteristic function W may be written in the form

$$W(\alpha,\mathbf{q})=\sum_{i=1}^{D} W_i(\alpha_1,\ldots,\alpha_D,q_i), \tag{2.4}$$

where the α_i are constants (generalized momenta), and W_k depends only on the conjugate coordinate q_k. The HJ equation then assumes the form

$$H=\sum_{i=1}^{D} H_i\left(\frac{\partial W_i}{\partial q_i},q_i\right)=\overline{E}, \tag{2.5}$$

which separates into the following one-dimensional problems:

$$H_i\left(\frac{\partial W_i}{\partial q_i},q_i\right)=H_i(p_i,q_i)=\overline{E}_i, \quad i=1,\ldots,D, \tag{2.6}$$

where the $\overline{E}_i$ are constants satisfying the restriction

$$\sum_{i=1}^{D} \overline{E}_i=\overline{E}. \tag{2.7}$$

We consider motion that is periodic in each of the one-dimensional problems in (2.6), i.e., $p_i(t)$ and $q_i(t)$ are periodic functions of time with period T_i that trace out a closed orbit Γ_i in the $p_i q_i$ plane. The corresponding action variables will be defined as

$$J_i=\frac{1}{2\pi}\oint_{\Gamma_i}\frac{\partial W_i}{\partial q_i}\,dq_i=\frac{1}{2\pi}\oint_{\Gamma_i} p_i\,dq_i. \tag{2.8}$$

In the case of one-space-dimensional periodic motion about a potential minimum, as depicted in Fig. 1, J is (up to a normalization by 2π) the area in the pq phase space enclosed by a periodic orbit Γ. For the classical one-dimensional harmonic oscillator,

$$H=\frac{p^2}{2m}+\frac{1}{2}m\omega^2x^2, \tag{2.9}$$

this leads to the well-known result

$$\overline{E}=\omega J. \tag{2.10}$$

The perturbed problems and canonical perturbation theory

The perturbation problems to be studied will have the form

$$H(\mathbf{p},\mathbf{q})=H^{(0)}(\mathbf{p},\mathbf{q})+\lambda W(\mathbf{q}), \tag{2.11}$$

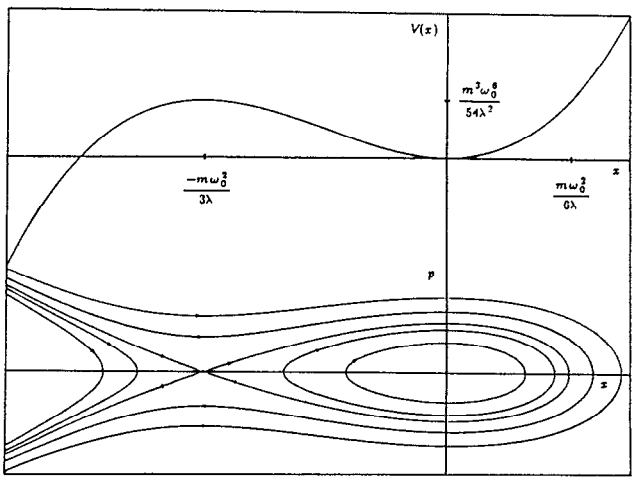

FIG. 2. Plot of potential energy function for the classical cubic anharmonic oscillator [$M=3$ in Eq. (2.12)], $V(x)=\frac{1}{2}m\omega_0^2x^2+\lambda x^3$ and corresponding phase portraits below.

where $H^{(0)}$ represents the "unperturbed" Hamiltonian, and W the perturbing potential. As usual, it is assumed that the dynamics associated with $H^{(0)}$ is exactly solvable, e.g., harmonic oscillator, Kepler problem. As an example, consider the general one-dimensional anharmonic oscillator problems:

$$H(p,x)=\frac{p^2}{2m}+\frac{1}{2}m\omega_0^2x^2+\lambda x^M, \quad M=1,2,\ldots. \tag{2.12}$$

The two sketches in Figs. 1(a) and 1(b) represent phase portraits for the perturbing potential $W(x)=x^4$, for (i) $\lambda>0$ and (ii) $\lambda<0$, respectively. The case $W(x)=x^3$ is depicted in Fig. 2.

Canonical perturbation theory, often referred to as the Poincaré–von Zeipel method, is based on the action-angle formalism. For a detailed discussion, the reader is referred to Goldstein[1] (which, in turn, is discussed in Refs. 2 and 3). The essence of the method is as follows. It is first assumed that the action–angle variables (J_0,θ_0) are known for the unperturbed problem, i.e.,

$$H^{(0)}(p,q)=K^{(0)}(J_0), \quad \theta_0=\omega_0 t+\beta_0. \tag{2.13}$$

These variables constitute a valid set of canonical variables for any one-dimensional Hamiltonian but will *not* serve as the action-angle variables for the perturbed problem. Let the latter be denoted as (J,θ). The goal is to find the canonical transformation $(J_0,\theta_0)\rightarrow(J,\theta)$, specifically its generator $Y(J,\theta_0)$. The perturbed problem is then written as

$$H^{(0)}(p,q)+\lambda W(q)=K^{(0)}(J_0)+\lambda K^{(1)}(J_0,\theta_0)$$
$$=\bar{E}(J,\lambda), \tag{2.14}$$

with transformation equations

$$J_0=\frac{\partial Y}{\partial \theta_0}, \quad \theta=\frac{\partial Y}{\partial J}. \tag{2.15}$$

It is now assumed that the generator Y admits a power series expansion in λ as well as the energy $E(J,\lambda)$:

$$\bar{E}(J,\lambda)=\bar{E}^{(0)}(J)+\lambda\bar{E}^{(1)}(J)+\lambda^2\bar{E}^{(2)}(J)+\cdots. \tag{2.16}$$

The Hamilton–Jacobi equation for the perturbed system now becomes

$$K^{(0)}\left(\frac{\partial Y}{\partial\theta_0}\right)+\lambda K^{(1)}\left(\frac{\partial Y}{\partial\theta_0},\theta_0\right)=\bar{E}^{(0)}(J)+\lambda\bar{E}^{(1)}(J)+\cdots. \tag{2.17}$$

It is also important to note that the $K^{(i)}$, which are λ dependent, are expanded in a Taylor series in J_0 about the value $J_0=J$.

The canonical perturbation method, although ingenious, is very tedious, involving detailed manipulations and Fourier expansions. When applied to the cubic and quartic anharmonic oscillators given by $M=3$ and $M=4$, respectively, in Eq. (2.12), the following expansions are obtained for the energy:

Cubic AHO, $M=3$:

$$\bar{E}(J,\lambda)=\omega_0 J-\frac{15}{4}\frac{J^2}{m^3\omega_0^4}\lambda^2+\cdots, \tag{2.18a}$$

Quartic AHO, $M=4$:

$$\bar{E}(J,\lambda)=\omega_0 J+\frac{3}{2}\frac{J^2}{m^2\omega_0^2}\lambda-\frac{17}{4}\frac{J^3}{m^4\omega_0^5}\lambda^2+\cdots. \tag{2.18b}$$

These results will be useful for comparison with those of the simpler classical HVHF method discussed below.

There are two important points concerning these expansions, inherent in their derivation but not usually stressed in the literature. First, for a given value of the perturbation parameter λ, the energy series $\bar{E}(J,\lambda)$ converges to the energy of a classical orbit of the perturbed Hamiltonian whose action is *precisely* J. In other words, as λ is varied, the perturbation method tracks a *single* classical orbit Γ_λ with *fixed* classical action J.

Second, this "action fixing" plays a role in the radius of convergence R of the $\bar{E}(J,\lambda)$ expansion. For a fixed action J, R will be determined by the singularity lying closest to $\lambda=0$. Intuitively, one would expect such singularities to occur when a periodic orbit of action J can no longer be supported by the potential. As an example, we consider the even-parity anharmonic oscillator Hamiltonians, $M=2P$, $P=2,3,\ldots$, in (2.12). As λ is varied, the possible situations involving a periodic orbit with fixed action $J>0$ are captured in Fig. 1. (i) A periodic orbit with action $J>0$ can be supported for all $\lambda>0$ [Fig. 1(a)]. (ii) For $\lambda<0$, as $|\lambda|$ increases, the heights of the potential barriers defining the classical potential well decrease [Fig. 1(b)]. (iii) There will be a critical value $\lambda_c(J)$ at which the area enclosed by the separatrices (heteroclinic orbits) connecting the two barrier maxima (unstable hyperbolic equilibria) will be equal to J. We expect $R(J)=|\lambda_c(J)|$ to be the radius of convergence of the $\bar{E}(J,\lambda)$ expansion. From the nature of the potentials considered here, $R(J)$ will be inversely proportional to J. The situation is slightly different for the case where M is odd: for λ of either sign, there exists a potential maximum whose height and distance from the origin decrease as $|\lambda|$ increases. As a result, by increasing $|\lambda|$, a periodic orbit with action J will eventually be destroyed and replaced by a separatrix/homoclinic orbit. The situation for $M=3$ is shown in Fig. 2.

The radii of convergence corresponding to an action J are known in closed form for the cubic and quartic anharmonic oscillator potentials, as shown below. For the quartic case, $M=4$ in Eq. (2.12), the picture in Fig. 1 holds, and the radius of convergence of the series in (2.18b) is

$$R=|\lambda_c|=\frac{m^2\omega_0^3\sqrt{2}}{6\pi J}. \tag{2.19}$$

This result agrees (after a rescaling) with that of Turchetti.[14] For the cubic case, $M=3$, we find

$$R=|\lambda_c|=\frac{m^{3/2}\omega_0^{5/2}}{(15\pi J)^{1/2}}. \tag{2.20}$$

Finally, it is also interesting to consider the relationship between canonical perturbation theory and the variety of standard (noncanonical) perturbation methods for differential equations. This aspect is rarely addressed in the literature. A connection between the canonical, Poincaré–von Zeipel method and the (Poincaré–Linstedt) method of strained coordinates is shown by example in the Appendix A.

B. The quantum case

Given a classical Hamiltonian in (2.1), we now consider its quantum mechanical counterpart, the linear operator $\hat{H}(\hat{\mathbf{p}},\hat{\mathbf{q}})$ obtained from the following standard substitutions: $p_i\to\hat{p}_i=-i\hbar(\partial/\partial q_i)$, $q_i\to\hat{q}_i=q_i$. The result is the linear operator

$$\hat{H}(\hat{\mathbf{p}},\hat{\mathbf{q}})=\frac{1}{2m}\sum_{i=1}^{D}\hat{p}_i^2+\hat{V}(\hat{\mathbf{q}})$$

$$=-\frac{\hbar^2}{2m}\sum_{i=1}^{D}\frac{\partial^2}{\partial q_i^2}+V(q_1,\ldots,q_D). \tag{2.21}$$

The Hamiltonian $\hat{H}$ is assumed to be a self-adjoint linear operator on a Hilbert space $\mathscr{H}$ of functions, e.g., $\mathscr{L}^2(\mathbf{R}^D,dx)$. The inner product on $\mathscr{H}$ will be denoted by $\langle f,g\rangle, f,g\in\mathscr{H}$. Self-adjointness of $\hat{H}$ implies that $\langle f,\hat{H}g\rangle=\langle\hat{H}f,g\rangle$, $\forall f,g\in\mathscr{D}(\hat{H})$, where $\mathscr{D}(\hat{H})$ denotes the domain of $\hat{H}$ [closure $(\mathscr{D}(\hat{H}))=\mathscr{H}$]. A "complete" description of the quantum mechanical system is provided by the wave function $\Psi\in\mathscr{H}$ whose time evolution is determined by the time-dependent Schrödinger equation

$$i\hbar\frac{\partial\Psi}{\partial t}=\hat{H}\Psi. \tag{2.22}$$

The Hamiltonians $\hat{H}$ considered here are assumed not to depend explicitly on time. A separation of time and space variables may then be used to obtain the standard result

$$\Psi(\mathbf{q},t)=\psi(\mathbf{q})e^{-iEt/\hbar}, \tag{2.23}$$

where $\psi(\mathbf{q})\in\mathscr{H}$ is a solution of the corresponding time-independent Schrödinger equation

$$\hat{H}\psi=E\psi. \tag{2.24}$$

It will be assumed that ψ is normalized, i.e., $\langle\psi,\psi\rangle=1$.

As a recurring example, the quantum mechanical counterpart of the classical one-dimensional harmonic oscillator in (2.9) is given by the Hamiltonian

$$\hat{H}=-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}+\frac{1}{2}m\omega^2x^2, \tag{2.25}$$

with eigenvalues

$$E_N=(N+\tfrac{1}{2})\hbar\omega,\quad N=0,1,2,\ldots, \tag{2.26}$$

and associated eigenfunctions

$$\psi_N(x)=(2^N N!)^{-1/2}\left(\frac{\alpha}{\pi}\right)^{1/4}e^{-\alpha x^2/2}H_N(\alpha^{1/2}x),$$

$$\alpha=\frac{m\omega}{\hbar}, \tag{2.27}$$

where $H_N(x)$ denotes the Hermite polynomial of degree N.

The perturbed problems

In correspondence with the classical perturbation problems in (2.11), we consider perturbed time-independent Hamiltonians of the form

$$\hat{H}=\hat{H}^{(0)}+\lambda\hat{W}, \tag{2.28}$$

where $\hat{H}^{(0)}$ and $\hat{W}$ denote "unperturbed" and "perturbation" operators, respectively. (The extension to Hamiltonians with higher powers of the coupling constant λ is straightforward.) It is assumed that both operators are Hermitian and that $\hat{H}^{(0)}$ possesses a complete set of orthonormal eigenfunctions $\phi_N^{(0)}$ (N may be an integer or a vector of integers) with distinct eigenvalues $E_N^{(0)}$,

$$\hat{H}^{(0)}\phi_N^{(0)}=E_N^{(0)}\phi_N^{(0)}. \tag{2.29}$$

Standard Rayleigh–Schrödinger perturbation theory (RSPT)[29] assumes that the eigenvalues of the perturbed Schrödinger equation,

$$\hat{H}\psi_N=E_N\psi_N, \tag{2.30}$$

admit series expansions of the form

$$E_N=E_N(\lambda)=\sum_{n=0}^{\infty}E_N^{(n)}\lambda^n. \tag{2.31}$$

(The associated expansions for the wave functions are not of interest here.) It is well known that the eigenvalue expansions (2.31) encountered in nonrelativistic quantum mechanics are typically divergent, yet asymptotic, to $E(\lambda)$ in some sector of the complex λ plane. The large-order behavior of the RSPT coefficients $E^{(n)}$ is generally given by[30,31]

$$E^{(n)}\sim(-1)^{n+1}A\Gamma(Bn+C)D^n[1+o(1)],\quad n\to\infty, \tag{2.32}$$

where A,B,C,D are constants specific to the problem (and quantum state) studied. In many cases, $E(\lambda)$ is analytic in an appropriate sector of the plane which includes the positive λ axis, and Borel or Padé summability of the RSPT series can be established.[32]

A special relationship exists between the quantum RSPT series for an eigenvalue $E(\lambda)$ and the canonical series for the energy $\bar{E}(J,\lambda)$ of the corresponding classical problem. Turchetti[14] first demonstrated this feature for the one-dimensional quartic anharmonic oscillator. The result was rigorously extended by Graffi and Paul,[15] as summarized below.

Consider the D-dimensional unperturbed oscillator Hamiltonians having the form

$$\hat{H}^{(0)}=\sum_{k=1}^{D}\left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x_k^2}+\frac{1}{2}m\omega_k^2x_k^2\right), \tag{2.33}$$

with nonresonant frequencies, i.e., there exists no nonzero vector of integers $\mathbf{N}=(N_1,N_2,...,N_D)\in\mathbf{Z}^D$ such that

$$\sum_{k=1}^{D}N_k\omega_k=0. \tag{2.34}$$

The eigenvalues of $\hat{H}^{(0)}$ will be denoted as

$$E^{(0)}(\mathbf{N},\hbar)=\sum_{k=1}^{D}\left(N_k+\frac{1}{2}\right)\hbar\omega_k, \tag{2.35}$$

where the explicit dependence on $\hbar$ and the quantum numbers $\mathbf{N}$ has been indicated. Let

$$\hat{H}=\hat{H}^{(0)}+\lambda\hat{W}(\mathbf{q}) \tag{2.36}$$

denote the perturbed Hamiltonian, where W is an entire function. The eigenvalues $E(\mathbf{N},\hbar,\lambda)$ of $\hat{H}$ are assumed to admit the following RS expansions:

$$E(\mathbf{N},\hbar,\lambda)=\sum_{n=0}^{\infty}E^{(n)}(\mathbf{N},\hbar)\lambda^n. \tag{2.37}$$

Now consider the associated classical perturbed Hamiltonian $H(\mathbf{p},\mathbf{q})$, which admits the following canonical series:

$$\overline{E}(\mathbf{J},\lambda)=\sum_{n=0}^{\infty}\overline{E}^{(n)}(\mathbf{J})\lambda^n, \tag{2.38}$$

where $\mathbf{J}=(J_1,...,J_D)$. If the following classical limit is taken, $N_i\to\infty$, $\hbar\to0$, such that $N_i\hbar=J_i$, $i=1,2,...,D$, then the following relation exists between the quantum and classical series coefficients:

$$E^{(n)}(\mathbf{N},\hbar)\underset{N_i\hbar=J_i}{\overset{\substack{N_i\to\infty\\ \hbar\to0}}{\to}}\overline{E}^{(n)}(\mathbf{J}),\quad n=0,1,2,\ldots. \tag{2.39}$$

This classical limit is trivially demonstrated for the unperturbed energies of separable harmonic oscillators. In the one-dimensional case, we may compare the classical energies in (2.10) with the quantum eigenvalues in (2.26). (The correspondence of higher-order coefficients will be demonstrated in Sec. V. As well, this classical limit relation will also be shown for perturbed hydrogenic problems.)

A deeper connection between quantum and classical perturbation expansions was revealed by Alvarez, Graffi, and Silverstone[16,17] in their detailed study of the 1-D quartic and cubic anharmonic oscillators. For the quartic case, each RS coefficient in (2.37) may be written in the form

$$E^{(n)}(N,\hbar)=\hbar^{n+1}\sum_{k=0}^{n+1}a_k^{(n)}\left(N+\frac{1}{2}\right)^k. \tag{2.40}$$

(The general result for 1-D anharmonic oscillators will be derived in Sec. V A below.) Substitution into (2.37) and rearrangement leads to the result

$$E(N,\hbar,\lambda)=\overline{E}(J,\lambda)+\sum_{n=1}^{\infty}\hbar^{2n}\overline{E}_{2n}(J,\lambda). \tag{2.41}$$

Thus, the RS series in (2.37) may be written as the sum of the classical series in (2.38) plus an infinite series of "quantum corrections" in powers of $\hbar$. Moreover, the perturbation expansion in λ for each correction $\overline{E}_{2n}(J,\lambda)$ is convergent, with radius of convergence equal to that of the classical series $\overline{E}(J,\lambda)$. This is extremely interesting in light of the fact that the fully quantum series $E(N,\hbar,\lambda)$ has zero radius of convergence.

III. THE QUANTUM MECHANICAL HV AND HF THEOREMS AND HVHF PERTURBATION THEORY

A. QM hypervirial theorem

Hirschfelder[5] introduced the classical hypervirial theorem, a generalization of the well-known virial theorem. In this paper, he also derived the quantum mechanical hypervirial theorem from the Heisenberg equations of motion. The standard shorter proof, due originally to Epstein and Epstein,[33] is sketched below. For a comprehensive discussion of the virial and hypervirial theorems and their applications in both classical and quantum mechanics, the reader is referred to the review article by Marc and McMillan,[34] as well as the monograph by Fernandez and Castro.[35]

Let $\hat{H}$ be time independent and self-adjoint with eigenfunction ψ, as in Eq. (2.24). Then, for any time-independent linear operator $\hat{O}$ on the space $\mathscr{H}$, the following expectation value vanishes:

$$\langle\psi,[\hat{O},\hat{H}]\psi\rangle=0, \tag{3.1}$$

where $[\hat{A},\hat{B}]=\hat{A}\hat{B}-\hat{B}\hat{A}$, provided that $\hat{H}$ is self-adjoint with respect to *both* the functions ψ and $\hat{O}\psi$. This result follows immediately from Eq. (2.24) and the self-adjointness of $\hat{H}$. For Hamiltonians of the form (2.21), where self-adjointness with respect to $\hat{O}\psi$ is not assumed, the above expectation value becomes

$$\langle\psi,[\hat{O},\hat{H}]\psi\rangle=\frac{\hbar^2}{2m}\int\int_S[\psi^*\nabla(\hat{O}\psi)-(\hat{O}\psi)\nabla\psi^*]\cdot d\mathbf{S}. \tag{3.2}$$

The self-adjointness condition involves the vanishing of this surface integral which, in turn, depends upon the boundary conditions of the problem. This aspect is rarely stressed in the standard textbooks. Fernandez and Cas-

tro[36] have taken this fact into account in the perturbation treatments of bounded quantum systems.

We illustrate the usefulness of this theorem with the relatively simple class of one-dimensional Hamiltonians

$$\hat{H}=-\frac{\hbar^2}{2m}\hat{D}_x^2+V(x), \quad \hat{D}_x\equiv\frac{d}{dx}. \tag{3.3}$$

If we choose $\hat{O}=x^k\hat{D}_x$, $k=1,2,...$, and evaluate the commutator in (3.1) explicitly, then a set of recursion relations involving the expectation values

$$\langle x^m\rangle\equiv\langle\psi,x^m\psi\rangle, \quad m=0,1,2,... \quad (\langle x^0\rangle=1), \tag{3.4}$$

are obtained. These relations are known as the *hypervirial relations*: in particular, the case $k=1$ corresponds to the usual *virial theorem*. In order to evaluate the commutators, the following relations are used:

$$[\hat{D}_x,\hat{H}]=\hat{D}_xV=\frac{dV}{dx}, \tag{3.5a}$$

$$[x^k,\hat{H}]=\frac{\hbar^2}{m}\left(kx^{k-1}\hat{D}_x+\frac{1}{2}k(k-1)x^{k-2}\right), \tag{3.5b}$$

as well as the operator identity

$$[x^k\hat{D}_x,\hat{H}]=x^k[\hat{D}_x,\hat{H}]+[x^k,\hat{H}]\hat{D}_x. \tag{3.5c}$$

The latter identity is used to rewrite the commutator in (3.1), while the appearances of $\hat{D}_x$ and $\hat{D}_x^2$ are eliminated with the use of (3.5b) and the time-independent Schrödinger equation (2.24). Taking expectation values with respect to an eigenstate ψ with energy E yields the general hypervirial relations

$$2kE\langle x^{k-1}\rangle=2k\langle x^{k-1}V\rangle+\langle x^k\hat{D}_xV\rangle-(\hbar^2/4m)k \times(k-1)(k-2)\langle x^{k-3}\rangle, \quad k\in\mathbf{Z}. \tag{3.6}$$

In the case of solvable Hamiltonians, e.g., harmonic oscillator, (radial) hydrogenic atoms, these relations necessarily coincide with those obtained from a knowledge of the recursion relations between the orthogonal polynomials (Hermite, Laguerre, resp.) which comprise the eigenfunctions. For the one-dimensional harmonic oscillator, cf. (2.25)–(2.27), Eq. (3.6) produces the following recursion relations:

$$\langle x^{k+2}\rangle=\frac{2(k+1)}{k+2}\left(N+\frac{1}{2}\right)\left(\frac{\hbar}{m\omega}\right)\langle x^k\rangle +\frac{k(k-1)(k+1)}{4(k+2)}\left(\frac{\hbar}{m\omega}\right)^2\langle x^{k-2}\rangle. \tag{3.7}$$

The first three nonzero expectation values (the odd powers of x vanish) for the eigenstate ψ_N are given by

$$\langle x^2\rangle=\left(N+\frac{1}{2}\right)\left(\frac{\hbar}{m\omega}\right),$$

$$\langle x^4\rangle=\left(\frac{3}{2}N^2+\frac{3}{2}N+\frac{3}{4}\right)\left(\frac{\hbar}{m\omega}\right)^2, \tag{3.8}$$

$$\langle x^6\rangle=\left(\frac{5}{2}N^3+\frac{15}{4}N^2+5N+\frac{15}{8}\right)\left(\frac{\hbar}{m\omega}\right)^3.$$

B. QM Hellmann–Feynman theorem

In an interesting article about the origins of this theorem, Musher[37] attributes its first derivation to Pauli.[38] Hellmann[6a] and Feynman[6b] independently applied this theorem to the force concept in molecules by using the internuclear distance as a parameter.

Let $\hat{H}$ be a time-independent, self-adjoint operator that depends explicitly on a scalar parameter λ (representing, for example, mass, nuclear charge, or external magnetic field strength). In order to emphasize this dependence, we shall write $\hat{H}_\lambda$. Now assume that for a nontrivial range of λ values, there exist normalized eigenfunctions of H_λ, i.e.,

$$\hat{H}_\lambda\psi=E(\lambda)\psi, \quad \langle\psi,\psi\rangle=1. \tag{3.9}$$

The HF theorem states that

$$\frac{\partial E}{\partial\lambda}=\left\langle\psi,\frac{\partial\hat{H}_\lambda}{\partial\lambda}\psi\right\rangle. \tag{3.10}$$

The proof of (3.10) follows from a straightforward computation: differentiate $E(\lambda)=\langle\psi,\hat{H}_\lambda\psi\rangle$ with respect to λ to obtain

$$\frac{\partial E}{\partial\lambda}=\left\langle\frac{\partial\psi}{\partial\lambda},\hat{H}_\lambda\psi\right\rangle+\left\langle\psi,\left(\frac{\partial\hat{H}_\lambda}{\partial\lambda}\right)\psi\right\rangle+\left\langle\psi,\hat{H}_\lambda\frac{\partial\psi}{\partial\lambda}\right\rangle.$$

If $\hat{H}_\lambda$ is Hermitian with respect to ψ and $\partial\psi/\partial\lambda$, then this equation becomes

$$\frac{\partial E}{\partial\lambda}=E\left[\left\langle\frac{\partial\psi}{\partial\lambda},\psi\right\rangle+\left\langle\psi,\frac{\partial\psi}{\partial\lambda}\right\rangle\right]+\left\langle\psi,\frac{\partial\hat{H}_\lambda}{\partial\lambda}\psi\right\rangle.$$

The term in square brackets vanishes since the norm of ψ is constant, giving the desired result. As in the hypervirial theorem, complications arise if the hermicity property of $\hat{H}_\lambda$ with respect to both ψ and $\partial\psi/\partial\lambda$ is not satisfied, due to the appearance of a surface integral.[34] For Hamiltonians of the form in Eq. (2.21) this integral is given by

$$\left\langle \psi, \hat{H}_\lambda \frac{\partial \psi}{\partial \lambda} \right\rangle - \left\langle \hat{H}_\lambda \psi, \frac{\partial \psi}{\partial \lambda} \right\rangle$$

$$= \frac{\hbar^2}{2m} \int\int_S \left[\left(\frac{\partial \psi}{\partial \lambda} \right) \nabla(\psi^*) - \psi^* \nabla \left(\frac{\partial \psi}{\partial \lambda} \right) \right] \cdot d\mathbf{S}.$$

C. HVHF "perturbation theory without wave functions"

As mentioned in the Introduction, the use of the quantum mechanical hypervirial and Hellmann–Feynman theorems to provide Rayleigh–Schrödinger perturbation expansions is well known.[7,8] Our description of the HVHF perturbative method is brief and restricted to the one-dimensional case, where we need to consider only expectation values of the form (3.4). The first step in the treatment of perturbed Hamiltonians of the form (2.28) is to obtain the hypervirial relations (3.6) for $\langle x^k \rangle$ and E for a particular perturbed eigenstate. Next, the following series expansions are assumed:

$$E(\lambda) = \sum_{n=0}^{\infty} E^{(n)} \lambda^n, \tag{3.11a}$$

$$\langle x^k \rangle(\lambda) = \sum_{n=0}^{\infty} C_k^{(n)} \lambda^n. \tag{3.11b}$$

The unperturbed energy $E^{(0)}$ is known. As well, the normalization condition $\langle x^0 \rangle = 1$ is imposed, implying that

$$C_0^{(n)} = \delta_{0n}. \tag{3.12}$$

Substitution of these expansions into (3.6) and collecting like powers of λ^n yields a system of difference equations involving the $C_k^{(i)}$ and the $E^{(j)}$. However, this system is not closed, since the relation between these two sets of coefficients has not yet been defined. The closure is provided by the Hellmann–Feynman relation (3.10) which, in this case, becomes

$$\frac{\partial E}{\partial \lambda} = \langle \hat{W} \rangle. \tag{3.13}$$

The series for $E(\lambda)$ is formally differentiated and matched termwise in powers of λ with the series for $\langle \hat{W} \rangle$. Subject to conditions of analyticity of E and $\langle x^k \rangle$ in sectors of the complex λ-plane, the differentiation and termwise matching is rigorously justified in the context of asymptotic expansions.[39]

The $C_k^{(i)}$ array is generally calculated columnwise, starting from the $i=0$ (unperturbed) column, whose downward computation was already illustrated, cf. (3.7). Note that (3.11b) could be considered as a replacement of the usual expansion for $\psi(\lambda)$ in RSPT. A knowledge of the nth column in the $C_k^{(i)}$ array permits calculation of $E^{(n+1)}$, in analogy with RSPT using wave functions. Examples will be given in Sec. V.

IV. THE CLASSICAL HV AND HF THEOREMS AND HVHF PERTURBATION THEORY

A. Classical hypervirial theorem

We return to consider classical mechanical systems defined by the Hamiltonians in (2.1). Let $F(\mathbf{p},\mathbf{q})$ denote an arbitrary function of the dynamical variables, with no explicit time dependence, evaluated on a solution trajectory. Differentiating F with respect to time gives

$$\frac{dF}{dt} = \sum_{j=1}^{D} \left[\frac{\partial F}{\partial p_j} \dot{p}_j + \frac{\partial F}{\partial q_j} \dot{q}_j \right]$$

$$= \sum_{j=1}^{D} \left[-\frac{\partial F}{\partial p_j} \frac{\partial H}{\partial q_j} + \frac{\partial F}{\partial q_j} \frac{\partial H}{\partial p_j} \right]$$

$$= \{F,H\}, \tag{4.1}$$

where the braces denote the Poisson bracket. Now define the time average of a function $G(\mathbf{p},\mathbf{q})$ along a solution curve of Hamilton's equations as

$$\overline{G} = \lim_{\tau \to \infty} \frac{1}{\tau} \int_0^\tau G(\mathbf{p}(t),\mathbf{q}(t)) dt \tag{4.2}$$

for a nonperiodic orbit and

$$\overline{G} = \frac{1}{T} \int_0^T G(\mathbf{p}(t),\mathbf{q}(t)) dt \tag{4.3}$$

for a T-periodic orbit. Now consider the time average of $G = dF/dt$, assuming that the p_i, q_i, as well as $F(\mathbf{p},\mathbf{q})$, remain bounded for all values of time. Note that

$$\frac{1}{\tau} \int_0^\tau G\, dt = \frac{1}{\tau} \int_0^\tau \frac{dF}{dt} dt = \frac{1}{\tau} [F(\tau) - F(0)]. \tag{4.4}$$

The time average (4.3) of dF/dt for periodic motion automatically vanishes, since $\tau = T$ and $F(T) = F(0)$. The time average (4.2) of dF/dt for nonperiodic motion vanishes in the limit since the term in square brackets in (4.4) remains bounded, by hypothesis. Thus, from (4.1), we have the classical hypervirial theorem,[5]

$$\overline{\{F,H\}} = 0, \tag{4.5}$$

which may be considered a classical analogue of the quantum HV relation in (3.1).

For the Hamiltonians in (2.1), the generator

$$F(\mathbf{p},\mathbf{q})=\mathbf{q}\cdot\mathbf{p}=\sum_{i=1}^{D} q_i p_i \tag{4.6}$$

gives

$$\overline{\sum_{j=1}^{D} p_j\dot{q}_j}=-\overline{\sum_{j=1}^{D} q_j\dot{p}_j}. \tag{4.7}$$

From Hamilton's equations, (4.7) yields the classical virial theorem

$$2\overline{T}=\overline{\mathbf{q}\cdot\nabla V}, \tag{4.8}$$

where T denotes the kinetic energy, $\overline{E}=T+V$.

Consider now the one-dimensional Hamiltonians of the form (2.1). Using the generators $F(p,x)=x^k p$, $k\in\mathbf{Z}$, and the fact that $p^2=2m(E-V)$, the hypervirial relations in (4.5) become

$$2k\overline{Ex^{k-1}}=2k\overline{(x^{k-1}V)}+\overline{x^k(\hat{D}_x V)}, \quad k\in\mathbf{Z}. \tag{4.9}$$

These relations may be compared to their quantum mechanical counterparts in (3.6). For the one-dimensional harmonic oscillator, cf. (2.9), the recursion relations associated with a periodic orbit with action J are ($\overline{E}=J\omega$)

$$\overline{x^{k+2}}=2\frac{k+1}{k+2}\left(\frac{J}{m\omega}\right)\overline{x^k} \quad (\overline{x^0}=1), \tag{4.10}$$

so that the first three nonzero expectation values are

$$\overline{x^2}=\frac{J}{m\omega},$$

$$\overline{x^4}=\frac{3}{2}\left(\frac{J}{m\omega}\right)^2, \tag{4.11}$$

$$\overline{x^6}=\frac{5}{2}\left(\frac{J}{m\omega}\right)^3.$$

The classical limit demonstrated by perturbation theory is also seen to apply to expectation values: Comparing (4.11) to (3.8), $\langle x^{2k}\rangle \to \overline{x^{2k}}$ in the limit $N\to\infty$, $\hbar\to 0$, $N\hbar=J$. This feature may be explained in terms of the classical limit of the associated Wigner distribution function. For 1-D problems, the Wigner distribution P_W: $\mathbf{R}^2\to\mathbf{R}$ corresponding to an eigenstate ψ is given by[40]

$$P_W(p,q)=\frac{1}{\pi\hbar}\int_{-\infty}^{\infty}\psi^*(q+y)\psi(q-y)e^{2ipy/\hbar}\,dy. \tag{4.12}$$

By the Weyl correspondence, if $\hat{A}(\hat{p},\hat{q})$ is a quantum mechanical operator corresponding to a classical function $A(p,q)$, then

$$\langle\psi,\hat{A}\psi\rangle=\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}P_W(p,q)A(p,q)\,dp\,dq. \tag{4.13}$$

In the classical limit, it has been shown[41] that the Wigner function becomes a delta-function distribution on the torus with action J, i.e.,

$$P_{cl}(p,q)=\delta[J-J(p,q)]. \tag{4.14}$$

For the 1-D problems discussed above, this torus coincides exactly with the classical periodic orbit of action J.

B. Classical Hellmann–Feynman theorem

The classical HF theorem for periodic orbits follows from two fundamental principles of classical mechanics:[1,2,26] (i) Hamilton's principle and (ii) the principle of least action. We state the main features of each principle below, highlighting the assumptions made, and then proceed to prove the classical HF theorem.

First, recall the Lagrangian formulation for a classical system with D generalized coordinates, q_i, $i=1,2,\ldots,D$ and their respective generalized velocities $\dot{q}_i$, $i=1,2,\ldots,D$. The Lagrangian L has the form

$$L(\mathbf{q}(t),\dot{\mathbf{q}}(t),t)=T(\mathbf{q}(t),\dot{\mathbf{q}}(t),t)-V(\mathbf{q}(t),\dot{\mathbf{q}}(t),t), \tag{4.15}$$

where T and V denote, respectively, the kinetic and potential energies of the system. The evolution of the mechanical system is represented by a point $\mathbf{q}(t)$ moving in the N-dimensional configuration space. Let $t_1<t_2$, and consider the actual path taken by the system between these two times, which will be denoted as $\mathbf{q}^*(t)$. Each of the principles mentioned above is based on the stationarity of its own integral with respect to a particular variation of paths about $\mathbf{q}^*(t)$ in configuration space:

Hamilton's principle: δ-variation, where the varied paths start and end at the same time as $\mathbf{q}^*(t)$,

principle of least action: Δ-variation, where the transit times are allowed to differ on the varied paths.

In both cases, the variation about a path $\mathbf{q}(t)$ may be defined as

$$q_i(t,\alpha)=q_i(t,0)+\alpha\eta_i(t), \quad i=1,2,\ldots,D, \tag{4.16}$$

where α is an infinitesimal parameter that goes to zero on the actual path. The δ and Δ variations of a path are given by

$$\delta q_i(t)=q_i(t,\alpha)-q_i(t,0)=\alpha\eta_i(t), \tag{4.17}$$

$$\Delta q_i(t)=q_i(t+\Delta t,\alpha)-q_i(t,0). \tag{4.18}$$

Using the parametrization of (4.16), Eq. (4.18) becomes

$$\Delta q_i(t)=q_i(t+\Delta t,0)+\alpha\eta_i(t+\Delta t)-q_i(t,0). \tag{4.19}$$

Now expand the first and second terms of the right side of (4.19) in a Taylor series and keep only terms of first order in the small quantities Δt and α. Then the following relation exists between the two variations:

$$\Delta q_i(t) = \Delta t \dot{q}_i(t,0) + \alpha \eta_i(t) = \Delta t \dot{q}_i(t,0) + \delta q_i(t). \quad (4.20)$$

Hamilton's principle states that out of all possible paths in configuration space that a point can travel between times t_1 and t_2, the actual path satisfies the stationarity condition

$$\delta \int_{t_1}^{t_2} L(\mathbf{q}(t),\dot{\mathbf{q}}(t),t)dt = 0. \quad (4.21)$$

The result is that $\mathbf{q}^*(t)$ is a solution of the Euler–Lagrange equations:

$$\frac{\partial L}{\partial q_i} - \frac{d}{dt}\left(\frac{\partial L}{\partial \dot{q}_i}\right) = 0, \quad i = 1,2,...,D. \quad (4.22)$$

The principle of least action states that the following stationarity condition must hold about $\mathbf{q}^*(t)$:

$$\Delta S(t_1,t_2) = \Delta \int_{t_1}^{t_2} \sum_{i=1}^{D} p_i \dot{q}_i \, dt = 0. \quad (4.23)$$

Here $S(t_1,t_2)$ is (up to a 2π factor) the total *classical action* associated with the trajectory between the times t_1 and t_2. Three restrictions must also be imposed:

(i) L, hence H, does not depend explicitly upon time, so that H is conserved,

(ii) the variation in (4.23) is such that H is conserved on the varied paths as well as on the actual path $\mathbf{q}^*(t)$,

(iii) the Δq_i vanish at the endpoints. This condition will be satisfied for periodic orbits, since we may allow the transit time to vary so that H is kept constant along the trajectory.

Following McKinley,[10] the proof of the classical HF theorem rests on the condition that the classical action associated with a periodic orbit is kept constant under infinitesimal Δ-variation. Let H be a time-independent Hamiltonian depending explicitly upon a parameter λ. Assume a λ value for which $H(\lambda)$ admits a family of periodic orbits. We consider one particular orbit Γ in this family that will correspond to the actual path $\mathbf{q}^*(t)$ discussed above. Let T be the period of Γ. The total variation of the classical action in (4.23) about Γ will be split into two parts:

(i) variation over nearby orbits, keeping the energy $\bar{E}$ and λ fixed;

(ii) parametric variation of λ, where $\bar{E} = \bar{E}(\lambda)$ is the energy of the orbit at the corresponding value of λ.

The stationarity condition of the classical action takes the form

$$\Delta \oint \sum_i p_i \, dq_i = \Delta \oint \sum_i p_i \, dq_i \Big|_{\lambda=\text{const}} + (\Delta\lambda) \frac{\partial}{\partial \lambda} \oint \sum_i p_i \, dq_i = 0. \quad (4.24)$$

By parametrizing each p_i and q_i as functions of t, the first term in (4.24) may be written as

$$\Delta \int_{t_1}^{t_2} \sum_i p_i \dot{q}_i \, dt \Big|_{\lambda=\text{const}} = 0, \quad (4.25)$$

where $t_2 = t_1 + T$. This is just a special case of the least action principle in (4.23). The first term in (4.24) will vanish provided that $\bar{E}$ is kept constant on Γ and on the varied paths and that Δq_i vanish at the endpoints. From our earlier discussions, the latter condition implies that the varied paths must be periodic.

The stationarity condition of the classical action now reduces to the following condition:

$$\frac{\partial}{\partial \lambda} \oint \sum_i p_i \, dq_i = 0. \quad (4.26)$$

Because we are considering only separable Hamiltonian systems, cf. Eq. (2.5), with purely periodic components, cf. Eq. (2.8), it suffices to prove the HF theorem for one-dimensional problems. We generalize Killingbeck's proof[42] for the quartic anharmonic oscillator to treat Hamiltonians of the form

$$H_\lambda = \frac{p_\lambda^2}{2m} + V_\lambda(x) = \bar{E}(\lambda). \quad (4.27)$$

Recall that the classical action of a periodic orbit $\Gamma \subset \mathbf{R}^2$ is equal to the area of its interior, i.e.,

$$\oint p dx = 2\sqrt{2m} \int_{x_1(\lambda)}^{x_2(\lambda)} (\bar{E}(\lambda) - V_\lambda(x))^{1/2} \, dx, \quad (4.28)$$

where $x_1(\lambda)$ and $x_2(\lambda)$ are the classical turning points. Taking the partial derivatives of both sides of (4.28) and imposing (4.26) implies that

$$(\bar{E}(\lambda)-V_\lambda(x_2))^{1/2}\frac{\partial x_2}{\partial\lambda}-(\bar{E}(\lambda)-V_\lambda(x_1))^{1/2}\frac{\partial x_1}{\partial\lambda}$$

$$+\frac{1}{2}\int_{x_1(\lambda)}^{x_2(\lambda)}\frac{(\partial\bar{E}/\partial\lambda-\partial V_\lambda/\partial\lambda)}{(\bar{E}-V_\lambda)^{1/2}}dx=0. \tag{4.29}$$

The first two terms vanish (classical turning point condition) so that (4.29) becomes

$$\frac{\partial\bar{E}}{\partial\lambda}=\frac{\int_{x_1}^{x_2}\partial V_\lambda/\partial\lambda\,(\bar{E}-V_\lambda)^{-1/2}\,dx}{\int_{x_1}^{x_2}(\bar{E}-V_\lambda)^{-1/2}\,dx}. \tag{4.30}$$

From Hamilton's equations, $\dot{x}=(2(\bar{E}-V_\lambda)/m)^{1/2}$ and Eq. (4.30) can be rewritten as

$$\frac{\partial\bar{E}}{\partial\lambda}=\frac{1}{T}\int_0^T\frac{\partial V_\lambda}{\partial\lambda}dt\equiv\overline{\frac{\partial V_\lambda}{\partial\lambda}}, \tag{4.31}$$

which is the desired result.

We may now return to consider the multidimensional case, cf. Eqs. (2.5)–(2.7). Since the component one-dimensional problems are independent, the HF theorem implies that

$$\frac{\partial}{\partial\lambda}\oint_{\Gamma_i}\frac{\partial W_i}{\partial q_i}dq_i=0,\quad i=1,2,...,D. \tag{4.32}$$

Writing the individual one-dimensional problems in the same form as Eq. (4.27) (omitting the explicit reference to λ),

$$H_i=\frac{p_i^2}{2m}+V_i(q_i)=\bar{E}_i(\lambda),\quad i=1,2,...,D, \tag{4.33}$$

then it follows that

$$\frac{\partial\bar{E}_i}{\partial\lambda}=\overline{\frac{\partial V_i}{\partial\lambda}},\quad i=1,2,...,D. \tag{4.34}$$

C. Classical HVHF "perturbation theory without Fourier series/differential equations"

We now arrive at the reformulation of canonical perturbation theory in terms of the classical HV and HF theorems. The classical HVHF perturbative method will be quite analogous to the quantum case in Sec. III C. Again, only the one-dimensional case need be discussed. Let Γ_0 denote an "unperturbed" classical orbit with action J and energy $\bar{E}^{(0)}(J)$. Assume that there exists a neighborhood N_ϵ of $\lambda=0$, such that for $\lambda\in N_\epsilon$, there exists a classical orbit Γ_λ with fixed action J and energy $\bar{E}(J,\lambda)$, so that Γ_λ may be considered a perturbation of Γ_0. Once the classical hypervirial relations for Hamiltonians of the form (2.11) are obtained, we assume the series expansions

$$\bar{E}(J,\lambda)=\sum_{n=0}^{\infty}\bar{E}^{(n)}(J)\lambda^n, \tag{4.35a}$$

$$\overline{x^k}(J,\lambda)=\sum_{n=0}^{\infty}\bar{C}_k^{(n)}(J)\lambda^n, \tag{4.35b}$$

associated with the orbits, Γ_λ, along with the normalization condition $\overline{x^0}=1$, implying that $\bar{C}_0^{(n)}=\delta_{0n}$. As in the quantum case, substitution of the above power series into the hypervirial relations, as well as the classical Hellmann–Feynman condition

$$\frac{\partial\bar{E}}{\partial\lambda}=\bar{W}, \tag{4.36}$$

provides a set of recursion relations which uniquely defines the $\bar{C}_k^{(i)}$ and the $\bar{E}^{(j)}(J)$. The construction of the C table will proceed in the same way as for the quantum case: downward and columnwise, beginning with the $i=0$ (unperturbed) column.

We finally emphasize: *The constancy of the classical action J implied by the Hellmann–Feynman theorem explains why the classical HVHF series coincides with the canonical perturbation series obtained by the Poincaré–von Zeipel method.*

V. APPLICATIONS

In the examples below, for clarity of notation, quantum numbers and action variables will be represented by upper case indices, e.g., $N,L,...$, in order that they may be distinguished from summation or order indices.

A. One-dimensional anharmonic oscillators

In this section we consider the eigenvalue expansions afforded by both classical and quantum HVHF methods as applied to the anharmonic oscillators. The quantum Hamiltonians considered are

$$\hat{H}=-\frac{\hbar^2}{2m}\hat{D}_x^2+\frac{1}{2}m\omega^2x^2+\lambda x^M,\quad M=1,2,..., \tag{5.1}$$

whose eigenvalue expansions will be written in the following form:

$$E(n,\hbar,\lambda)=\sum_{n=0}^{\infty}E^{(n)}(N,\hbar)\lambda^n,\quad N=0,1,2,..., \tag{5.2a}$$

$$E^{(0)}(N,\hbar)=(N+\tfrac{1}{2})\hbar\omega. \tag{5.2b}$$

The expectation values associated with the corresponding eigenstate will also be expanded as

$$\langle x^k\rangle(N,\hbar,\lambda)=\sum_{n=0}^{\infty}C_k^{(n)}(N,\hbar)\lambda^n. \tag{5.3}$$

The corresponding classical Hamiltonians are given by

$$H(p,x)=\frac{p^2}{2m}+\frac{1}{2}m\omega^2x^2+\lambda x^M,\quad M=1,2,3,..., \tag{5.4}$$

with associated energy expansions

$$\overline{E}(J,\lambda)=\sum_{n=0}^{\infty}\overline{E}^{(n)}(J)\lambda^n,\quad J>0, \tag{5.5a}$$

$$\overline{E}^{(0)}(J)=\omega J, \tag{5.5b}$$

and expectation values (time averages over periodic orbits)

$$\overline{x^k}(J,\lambda)=\sum_{n=0}^{\infty}\overline{C}_k^{(n)}(J)\lambda^n. \tag{5.6}$$

Quantum HVHF

For practical purposes of (especially symbolic) computation, it is convenient to work with the scaled oscillator Hamiltonians

$$\hat{H}_{sc}=-\hat{D}_X^2+X^2+\beta X^M, \tag{5.7}$$

with associated eigenvalue and expectation series

$$F(N,\beta)=\sum_{n=0}^{\infty}F^{(n)}(N)\beta^n,\quad F^{(0)}(N)=2N+1, \tag{5.8}$$

$$\langle X^k\rangle(N,\beta)=\sum_{n=0}^{\infty}D_k^{(n)}(N)\beta^n. \tag{5.9}$$

This is accomplished with the (unitary) transformation $x=\alpha X$, $\alpha=(\hbar/(m\omega))^{1/2}$. As a result

$$\beta=\frac{2}{\hbar\omega}\left(\frac{\hbar}{m\omega}\right)^{M/2}\lambda,\quad F(N,\beta)=\frac{2}{\hbar\omega}E(N,\hbar,\lambda). \tag{5.10}$$

The coefficients of "scaled" and "unscaled" expansions are related as follows:

$$E^{(n)}(N,\hbar)=\left(\frac{2}{\hbar\omega}\right)^{n-1}\left(\frac{\hbar}{m\omega}\right)^{Mn/2}F^{(n)}(N), \tag{5.11a}$$

$$C_k^{(n)}(N,\hbar)=\left(\frac{2}{\hbar\omega}\right)^{n}\left(\frac{\hbar}{m\omega}\right)^{(Mn+k)/2}D_k^{(n)}(N). \tag{5.11b}$$

Using the generator $\hat{O}=X^k\hat{D}_X$, the quantum hypervirial relations (3.6) for the scaled problem become

$$\begin{aligned}2(k+1)F\langle X^k\rangle=&\,2(k+2)\langle X^{k+2}\rangle+\beta(M+2k+2)\\&\times\langle X^{k+M}\rangle-\tfrac{1}{2}k(k-1)\\&\times(k+1)\langle X^{k-2}\rangle,\quad k\in\mathbf{Z}.\end{aligned} \tag{5.12}$$

From the Hellmann–Feynman theorem, $\partial F/\partial\beta=\langle X^M\rangle$. The following recurrence relations are obtained for the series coefficients in (5.11a) and (5.11b) (omitting explicit reference to the quantum number N):

$$\begin{aligned}kD_k^{(n)}=&(k-1)\sum_{j=0}^{n}F^{(j)}D_{k-2}^{(n-j)}-\frac{1}{2}(M+2k-2)\\&\times D_{M+k-2}^{(n-1)}+\tfrac{1}{4}(k-1)(k-2)(k-3)D_{k-4}^{(n)},\end{aligned} \tag{5.13}$$

$$F^{(n+1)}=\frac{1}{n+1}D_M^{(n)}. \tag{5.14}$$

The $D_k^{(n)}$ array may be computed columnwise, starting with the first column, $D_k^{(0)}$, $k=0,1,2,...$, which corresponds to the unperturbed problem. A knowledge of the nth column determines $F^{(n+1)}$. The absence of the constants $\hbar$, m, and ω facilitates computation of the series coefficients $E^{(n)}$. It also provides a clear understanding of the nature of the RS coefficients, as shown below.

Lemma: The scaled RS coefficients $F^{(n)}(N)$ in (5.8) behave as follows:

(i) For both M and n odd, $F^{(n)}(N)=0$.

(ii) Otherwise, they are polynomials in N of degree $\frac{1}{2}(M-2)n+1$, i.e.,

$$F^{(n)}(N)=\sum_{k=0}^{(1/2)(M-2)n+1}a_k^{(n)}N^k. \tag{5.15}$$

This Lemma may be proved by induction. From (5.11a) it follows that in the canonical classical limit of Sec. II B [cf. Eq. (2.39)], the RS coefficients for $E(N,\lambda)$ become

$$\begin{aligned}E^{(n)}(N,\hbar)\underset{N\hbar=J}{\overset{N\to\infty}{\hbar\to 0}}&\,\overline{E}^{(n)}(J)\\=&\left(\frac{2}{\omega}\right)^{n-1}\left(\frac{1}{m\omega}\right)^{Mn/2}\\&\times a_{(1/2)(M-2)n+1}^{(n)}J^{(1/2)(M-2)n+1}.\end{aligned} \tag{5.16}$$

The RS expansions for the cases $M=3$, 4 and 6 are shown in Table I. In each case, the first few terms of the series for $\langle x\rangle$ and $\langle x^2\rangle$ are also shown. (The cases $M=1,2$ represent test cases for which the eigenvalues,

TABLE I. RSPT series for quantum anharmonic oscillators with Hamiltonians of the form $\hat{H}=-(\hbar^2/2m)\,d^2/dx^2+(m\omega^2/2)\,x^2+\lambda x^M$.

M=3

$$E=\hbar\omega\left(N+\frac{1}{2}\right)-\frac{\hbar^2}{m^3\omega^4}\left(\frac{15}{4}N^2+\frac{15}{4}N+\frac{11}{8}\right)\lambda^2-\frac{\hbar^3}{m^6\omega^8}\left(\frac{705}{16}N^3+\frac{2115}{32}N^2+\frac{1635}{32}N+\frac{465}{32}\right)\lambda^4+\cdots$$

$$\langle x\rangle=-\frac{\hbar}{m^2\omega^3}\left(3N+\frac{3}{2}\right)\lambda-\frac{\hbar^2}{m^5\omega^8}\left(45N^2+45N+\frac{33}{2}\right)\lambda^3-\frac{\hbar^3}{m^8\omega^{13}}\left(\frac{19035}{16}N^3+\frac{57105}{32}N^2+\frac{44145}{32}N+\frac{12555}{32}\right)\lambda^5+\cdots$$

$$\langle x^2\rangle=\frac{\hbar}{m\omega}\left(N+\frac{1}{2}\right)+\frac{\hbar^2}{m^4\omega^6}\left(15N^2+15N+\frac{11}{2}\right)\lambda^2+\frac{\hbar^3}{m^7\omega^{11}}\left(\frac{6345}{16}N^3+\frac{19035}{32}N^2+\frac{14715}{32}N+\frac{4185}{32}\right)\lambda^4+\cdots$$

M=4

$$E=\hbar\omega\left(N+\frac{1}{2}\right)+\frac{\hbar^2}{m^2\omega^2}\left(\frac{3}{2}N^2+\frac{3}{2}N+\frac{3}{4}\right)\lambda-\frac{\hbar^3}{m^4\omega^5}\left(\frac{17}{4}N^3+\frac{51}{8}N^2+\frac{59}{8}N+\frac{21}{8}\right)\lambda^2+\cdots$$

$$\langle x^2\rangle=\frac{\hbar}{m\omega}\left(N+\frac{1}{2}\right)-\frac{\hbar^2}{m^3\omega^4}\left(3N^2+3N+\frac{3}{2}\right)\lambda+\frac{\hbar^3}{m^5\omega^7}\left(\frac{85}{4}N^3+\frac{255}{8}N^2+\frac{295}{8}N+\frac{105}{8}\right)\lambda^2+\cdots$$

$$\langle x^4\rangle=\frac{\hbar^2}{m^2\omega^2}\left(\frac{3}{2}N^2+\frac{3}{2}N+\frac{3}{4}\right)-\frac{\hbar^3}{m^4\omega^5}\left(\frac{17}{2}N^3+\frac{51}{4}N^2+\frac{59}{4}N+\frac{21}{4}\right)\lambda+\frac{\hbar^4}{m^6\omega^8}\left(\frac{1125}{16}N^4+\frac{1125}{8}N^3+\frac{531}{2}N^2+\frac{3123}{16}N+\frac{999}{16}\right)\lambda^2+\cdots$$

M=6

$$E=\hbar\omega\left(N+\frac{1}{2}\right)+\frac{\hbar^3}{m^3\omega^3}\left(\frac{5}{2}N^3+\frac{15}{4}N^2+5N+\frac{15}{8}\right)\lambda-\frac{\hbar^5}{m^6\omega^7}\left(\frac{393}{16}N^5+\frac{1965}{32}N^4+\frac{3055}{16}N^3+225N^2+\frac{1441}{8}N+\frac{3495}{64}\right)\lambda^2+\cdots$$

$$\langle x^2\rangle=\frac{\hbar}{m\omega}\left(N+\frac{1}{2}\right)-\frac{\hbar^3}{m^4\omega^5}\left(\frac{15}{2}N^3+\frac{45}{4}N^2+15N+\frac{45}{8}\right)\lambda+\frac{\hbar^5}{m^7\omega^9}\left(\frac{2751}{16}N^5+\frac{13755}{32}N^4+\frac{21385}{16}N^3+1575N^2+\frac{10087}{8}N+\frac{24465}{64}\right)\lambda^2+\cdots$$

$$\langle x^4\rangle=\frac{\hbar^2}{m^2\omega^2}\left(\frac{3}{2}N^2+\frac{3}{2}N+\frac{3}{4}\right)-\frac{\hbar^4}{m^5\omega^6}\left(\frac{165}{8}N^4+\frac{165}{4}N^3+\frac{345}{4}N^2+\frac{525}{8}N+\frac{45}{2}\right)\lambda+\frac{\hbar^6}{m^8\omega^{10}}\left(\frac{8421}{16}N^6+\frac{25263}{16}N^5+\frac{399495}{64}N^4+\frac{315285}{32}N^3+\frac{394533}{32}N^2+\frac{490623}{64}N+\frac{138195}{64}\right)\lambda^2+\cdots$$

hence their series expansions, are known in closed form, since the Hamiltonians may be rewritten in solvable form.)

A few remarks on the properties of the quantum RS series for $E(\lambda)$ are in order here. For $M>2$, the series are known to be divergent. For M even, i.e., $M=2P$, $P=2,3,\ldots$, the large-order behavior of the series coefficients is given by the asymptotic relation in (2.32), where $B=P-1$, and A, C and D are constants that depend on P and the quantum number N of the eigenvalue.[30] The energy $E(\lambda)$ is analytic in the cut plane $|\arg(\lambda)|<\pi$.[32] The series are Borel summable for all $P\geqslant 2$,[43] and Padé summable for $P=2,3$.[32] Note also that in these cases, expectation values of odd powers of x vanish, $\langle x^{2l+1}\rangle=0$, $l=0,1,2,\ldots$. For $M=2P+1$, $P=1,2,\ldots$, the energy series coefficients do not alternate in sign and the series are not summable on the real λ-line. However, the series are summable on the imaginary λ-line.[44] (The potentials are unstable for both $\lambda<0$ and $\lambda>0$. If we let $\mu=i\lambda$, then the resulting series are summable for $\mu>0$.)

It is also interesting to consider the continued fraction (CF) representations of RS eigenvalue expansions which have the form

$$E(\lambda)=E^{(0)}+\lambda C(\lambda), \tag{5.17}$$

where

$$C(\lambda)=\frac{c_1}{1+}\,\frac{c_2\lambda}{1+}\,\frac{c_3\lambda}{1+}\cdots. \tag{5.18}$$

(For comprehensive treatments of the analytic theory of CFs, the reader is referred to Refs. 45 and 46. The properties of CFs most relevant to RSPT are discussed in Ref. 47.) The RS expansions for many standard perturbation problems, e.g., anharmonic oscillators, radially perturbed hydrogenic atoms, are negative Stieltjes for $n\geqslant 1$. This implies that $C(\lambda)$ is an S-fraction, i.e., all coefficients c_n are positive. Moreover, when the Stieltjes RS coefficients behave asymptotically as in Eq. (2.32), with $B=1,2,3,\ldots$, then

$$c_n=O(n^B), \quad \text{as } n\to\infty. \tag{5.19}$$

In particular, when $B=1$, then

$$c_n=\tfrac{1}{2}Dn+o(1), \quad \text{as } n\to\infty. \tag{5.20}$$

For $0\leqslant B\leqslant 2$, Carleman's condition[45,46] is satisfied, which is sufficient to guarantee convergence of $C(\lambda)$, hence Padé summability of the RS series. The CF representa-

tions of anharmonic oscillators and radially perturbed hydrogenic atoms have been explored in Refs. 47 and 48.

Classical HVHF

As for the quantum case, we consider the scaled classical Hamiltonians

$$H_{sc}=P^2+X^2+\beta X^M, \tag{5.21}$$

with associated expansions

$$\bar{F}(J,\beta)=\sum_{n=0}^{\infty}\bar{F}^{(n)}(J)\beta^n, \quad \bar{F}^{(0)}(J)=2J, \tag{5.22}$$

$$\overline{X^k}(J,\beta)=\sum_{n=0}^{\infty}\bar{D}_k^{(n)}(J)\beta^n. \tag{5.23}$$

[Note that the scaling used here, $x = X/\sqrt{m\omega}$, $p = \sqrt{m\omega}P$, represents a canonical transformation with generator $F_2 = \sqrt{m\omega}xP$ in Eq. (9)–(17) in Ref. 1.] The result is

$$\beta=\frac{2}{\omega}\left(\frac{1}{m\omega}\right)^{M/2}\lambda, \quad \bar{F}(J,\beta)=\frac{2}{\omega}\bar{E}(J,\lambda). \tag{5.24}$$

The relations between coefficients corresponding to unscaled and scaled problems are thus given by

$$\bar{E}^{(n)}(J)=\left(\frac{2}{\omega}\right)^{n-1}\left(\frac{1}{m\omega}\right)^{Mn/2}\bar{F}^{(n)}(J), \tag{5.25a}$$

$$\bar{C}_k^{(n)}(J)=\left(\frac{2}{\omega}\right)^{n}\left(\frac{1}{m\omega}\right)^{(Mn+k)/2}\bar{D}_k^{(n)}(J). \tag{5.25b}$$

Using the hypervirial generator X^kP in Eq. (4.5), the classical hypervirial relations (4.9) become [as expected from the corresponding quantum case, Eq. (5.12)]

$$2(k+1)\bar{F}\,\overline{X^k}=2(k+2)\overline{X^{k+2}}+\beta(M+2k+2)\overline{X^{k+M}}. \tag{5.26}$$

The HF theorem gives $\partial\bar{F}/\partial\beta = \overline{X^M}$. The recursion relation for the series coefficients in (5.22) and (5.23) are

$$k\bar{D}_k^{(n)}=(k-1)\sum_{j=0}^{n}\bar{F}^{(j)}\bar{D}_{k-2}^{(n-j)}-\frac{1}{2}(M+2k-2)\bar{D}_{M+k-2}^{(n-1)}, \tag{5.27}$$

$$\bar{F}^{(n+1)}=\frac{1}{n+1}\bar{D}_M^{(n)}. \tag{5.28}$$

These relations may be compared with their quantum counterparts in Eqs. (5.13) and (5.14). Energy and expectation value expansions for the cases $M=3$, 4, and 6 are presented in Table II. [The energy series may be compared to Eq. (2.18), the results of canonical perturbation theory.] A comparison with the quantum results in Table I shows that in the classical limit,

TABLE II. Canonical perturbation series for classical anharmonic oscillators with Hamiltonians of the form $H=(1/2m)\,p^2+(m\omega^2/2)\,x^2+\lambda x^M=E$.

M=3

$$\bar{E}=J\omega-\frac{15}{4}\frac{J^2}{m^3\omega^4}\lambda^2-\frac{705}{16}\frac{J^3}{m^6\omega^9}\lambda^4-\cdots$$

$$\bar{x}=\frac{-3J}{m^2\omega^3}\lambda-\frac{45J^2}{m^5\omega^8}\lambda^3-\frac{19035}{16}\frac{J^3}{m^8\omega^{13}}\lambda^5-\cdots$$

$$\overline{x^2}=\frac{J}{m\omega}+\frac{15J^2}{m^4\omega^6}\lambda^2+\frac{6345}{16}\frac{J^3}{m^7\omega^{11}}\lambda^4+\cdots$$

M=4

$$\bar{E}=J\omega+\frac{3J^2}{2m^2\omega^2}\lambda-\frac{17J^3}{4m^4\omega^5}\lambda^2+\cdots$$

$$\overline{x^2}=\frac{J}{m\omega}-\frac{3J^2}{m^3\omega^4}\lambda+\frac{85J^3}{4m^5\omega^7}\lambda^2+\cdots$$

$$\overline{x^4}=\frac{3J^2}{2m^2\omega^2}-\frac{17J^3}{2m^4\omega^5}\lambda+\frac{1125J^4}{16m^6\omega^8}\lambda^2-\cdots$$

M=6

$$\bar{E}=J\omega+\frac{5}{2}\frac{J^3}{m^3\omega^3}\lambda-\frac{393}{16}\frac{J^5}{m^6\omega^7}\lambda^2+\cdots$$

$$\overline{x^2}=\frac{J}{m\omega}-\frac{15}{2}\frac{J^3}{m^4\omega^5}\lambda+\frac{2751}{16}\frac{J^5}{m^7\omega^9}\lambda^2+\cdots$$

$$\overline{x^4}=\frac{3J^2}{2m^2\omega^2}-\frac{165}{8}\frac{J^4}{m^5\omega^6}\lambda+\frac{8421}{16}\frac{J^6}{m^8\omega^{10}}\lambda^2+\cdots$$

$$E^{(n)}(N,\hbar)\to\bar{E}^{(n)}(J), \tag{5.29a}$$

$$C_k^{(n)}(N,\hbar)\to\bar{C}_k^{(n)}(J), \quad n=0,1,2,..., \tag{5.29b}$$

as $N\to\infty$, $\hbar\to 0$, $N\hbar=J$.

The radii of convergence R of the expansions for $\bar{E}(J,\lambda)$ in the cases $M=3$ and $M=4$ are given by Eqs. (2.19) and (2.20), respectively. For several values of J, a "numerical ratio test" was performed, where the limits of the sequences $\{\bar{E}^{(n)}(J)/\bar{E}^{(n+1)}(J)\}$ were estimated using the Thiele–Padé method of extrapolation.[49] In all cases, the limit estimates agreed well with the theoretical values. As well, the same radii of convergence $R(J)$ were also calculated for the series expansions of the time averages $\overline{x^k}$.

Regarding the CF representations of the classical energy series,

$$\bar{E}(J,\lambda)=\bar{E}^{(0)}(J)+\lambda C(\lambda), \tag{5.30}$$

it is significant to note that in all cases $C(\lambda)$ is an S-fraction. Numerical ratio tests performed on the CF co-

efficients c_n show that they tend to a limit as $n \to \infty$, which is a consequence of the fact that the energy series have nonzero radii of convergence. In fact, we find that

$$c_n \to (4R(J))^{-1}, \quad \text{as } n \to \infty.$$

From Van Vleck's theorem,[45] this suggests that $\bar{E}(J,\lambda)$ is at least meromorphic on the complex λ-plane with branch cut on $(-\infty, -R(J))$. Then $C(\lambda)$ converges uniformly on compact subsets of this cut plane.

B. Double perturbation theory for one-dimensional anharmonic oscillators

Here we wish to show that the quantum and classical HVHF perturbative methods can be easily applied to treat problems with more than one coupling constant. For example, consider the quantum Hamiltonians of the form

$$\hat{H} = -\frac{\hbar^2}{2m}\hat{D}_x^2 + \frac{1}{2}m\omega^2 x^2 + \lambda x^{M_1} + \mu x^{M_2}, \tag{5.31}$$

where λ and μ may be considered as independent perturbation parameters. The quantum HV relations (3.6) become

$$\begin{aligned} 2kE(\lambda)\langle x^{k-1}\rangle = {} & m\omega^2(k+1)\langle x^{k+1}\rangle \\ & + \lambda(2k+M_1)\langle x^{k+M_1-1}\rangle \\ & + \mu(2k+M_2)\langle x^{k+M_2-1}\rangle \\ & - \frac{\hbar^2}{4m}k(k-1)(k-2)\langle x^{k-3}\rangle, \end{aligned} \tag{5.32}$$

and two HF relations now appear:

$$\frac{\partial E}{\partial \lambda} = \langle x^{M_1}\rangle, \quad \frac{\partial E}{\partial \mu} = \langle x^{M_2}\rangle. \tag{5.33}$$

It is now necessary to expand E and $\langle x^k\rangle$ in terms of double perturbation series:

$$E(N,\hbar,\lambda,\mu) = \sum_{m=0}^{\infty}\sum_{n=0}^{\infty} E^{(m,n)}(N,\hbar)\lambda^m\mu^n, \tag{5.34a}$$

$$\langle x^k\rangle(N,\hbar,\lambda,\mu) = \sum_{m=0}^{\infty}\sum_{n=0}^{\infty} C_k^{(m,n)}(N,\hbar)\lambda^m\mu^n. \tag{5.34b}$$

Once again, it is convenient to work with a scaled Hamiltonian, but the details will be omitted here. For the special case $M_1=3$, $M_2=4$, we obtain the following series for the energy eigenvalues:

$$\begin{aligned} E(N,\lambda,\mu) = {} & \left(N+\frac{1}{2}\right)\hbar\omega + \left(\frac{3}{2}N^2+\frac{3}{2}N+\frac{3}{4}\right)\left(\frac{\hbar}{m\omega}\right)^2\mu \\ & - \left(\frac{15}{4}N^2+\frac{15}{4}N+\frac{11}{8}\right)\frac{\hbar^2}{m^3\omega^4}\lambda^2 \\ & - \left(\frac{17}{4}N^3+\frac{51}{8}N^2+\frac{59}{8}N+\frac{21}{8}\right) \\ & \times \frac{\hbar^3}{m^4\omega^5}\mu^2 + \cdots. \end{aligned} \tag{5.35}$$

The classical HVHF perturbative method proceeds in a completely analogous fashion (details omitted here). As expected, the canonical series for the classical energy is found to be the appropriate limit of the series in (5.35), i.e.,

$$\bar{E}(J,\lambda,\mu) = \omega J + \frac{3J^2}{2m^2\omega^2}\mu - \frac{15J^2}{4m^3\omega^4}\lambda^2 - \frac{17J^3}{4m^4\omega^5}\mu^2 + \cdots. \tag{5.36}$$

These expansions agree with those obtained by Ali and Wood.[24(b),24(c)] The reader will also note the agreement of this series to lowest terms with the expansions in Eq. (2.18).

C. Central forces

1. The quantum case—radially perturbed hydrogenic atoms

We now consider eigenvalue/expectation value expansions of radially perturbed hydrogenic atoms. In D-dimensional space, a separation of variables $\psi(\mathbf{r}) = R(r)Y(\Omega)$ is performed to factor out the angular Ω-dependence in terms of D-dimensional spherical harmonics. The resulting radial eigenvalue equations will have the form

$$\begin{aligned} \hat{H}R_{NL}(r) = {} & \left[-\frac{\hbar^2}{2m}\left(\frac{d^2}{dr^2}+\frac{D-1}{r}\frac{d}{dr}-\frac{1}{r^2}L(L+D-2)\right)\right. \\ & \left. -\frac{b}{r}+\lambda r^Q\right]R_{NL}(r) \\ = {} & E(N,L,\hbar,\lambda)R_{NL}(r), \quad Q \in \mathbf{Z}. \end{aligned} \tag{5.37}$$

Here $b=Ze^2$, where Z represents the atomic number and e is the electronic charge. The indices N and L will represent the principal and angular quantum numbers, respectively. (The magnetic quantum number M plays no role here. Also, the L degeneracy of the unperturbed states is broken by the perturbation.) The scalar $L(L+D-2)$ denotes the eigenvalue of the square of the D-dimensional angular momentum operator.[50]

The hypervirial relations for the three-dimensional hydrogen atom were first studied by Killingbeck,[8] who formulated the HVHF perturbation method for this problem. It was subsequently employed by a number of workers to study various perturbations of the hydrogen atom, including screened Coulomb potentials[51] and the Stark effect.[52] The HV relations for D-dimensional atoms with arbitrary radial potentials $V(r)$ were derived in Ref. 48. Here, we shall apply the HVHF perturbation method to the standard case $D=3$. The eigenvalue expansion will be written as

$$E(N,L,\hbar,\lambda)=\sum_{n=0}^{\infty}E^{(n)}(N,L,\hbar)\lambda^n, \tag{5.38a}$$

$$E^{(0)}(N,L,\hbar)=-\frac{mb^2}{2N^2\hbar^2}. \tag{5.38b}$$

The expectation value expansions will be denoted as

$$\langle r^k\rangle(N,L,\hbar,\lambda)=\int_0^{\infty}R_{NL}^{*}(r)R_{NL}(r)r^2\,dr$$

$$=\sum_{n=0}^{\infty}C_k^{(n)}(N,L,\hbar)\lambda^n. \tag{5.39}$$

For practical purposes it is again convenient to work with the following scaled Hamiltonian, in which no physical constants appear:

$$\hat{H}_{sc}=-\hat{D}_R^2-\frac{2}{R}\hat{D}_R+\frac{L(L+1)}{R^2}-\frac{1}{R}+\beta R^Q. \tag{5.40}$$

The associated expansions are

$$F(N,L,\beta)=\sum_{n=0}^{\infty}F^{(n)}(N,L)\beta^n,$$

$$F^{(0)}(N,L)=-\frac{1}{4N^2},\quad N=1,2,..., \tag{5.41}$$

$$\langle R^k\rangle(N,L,\beta)=\sum_{n=0}^{\infty}D_k^{(n)}(N,L)\beta^n. \tag{5.42}$$

The Hamiltonians in (5.37) and (5.40) are related by the scaling transformation $r=\hbar^2R/(2mb)$, which implies that

$$\beta=\frac{\lambda}{b}\left[\frac{\hbar^2}{2mb}\right]^{Q+1},\quad E(N,L,\hbar,\lambda)=\frac{2mb^2}{\hbar^2}F(N,L,\beta), \tag{5.43}$$

so that

$$E^{(n)}(N,L,\hbar)=\frac{1}{b^{n-1}}\left(\frac{\hbar^2}{2mb}\right)^{Qn+n-1}F^{(n)}(N,L), \tag{5.44}$$

$$C_k^{(n)}(N,L,\hbar)=\frac{1}{b^n}\left(\frac{\hbar^2}{2mb}\right)^{Qn+n+k}D_k^{(n)}(N,L). \tag{5.45}$$

Using the generator $\hat{O}=R^k\hat{D}_R$, the quantum HV relations for the scaled problem become

$$2(k+1)F\langle R^k\rangle=-(2k+1)\langle R^{k-1}\rangle+\beta(2k+Q+2)\times\langle R^{k+Q}\rangle+2k[L(L+1)-\tfrac{1}{4}(k+1)\times(k-1)]\langle R^{k-2}\rangle,\quad k\in\mathbf{Z}. \tag{5.46}$$

From the Hellmann–Feynman theorem, $\partial F/\partial\beta=\langle R^Q\rangle$. The HVHF recurrence relations become (the quantum indices K,L will be supressed)

$$2(k+1)F^{(0)}D_k^{(0)}=-(2k+1)D_{k-1}^{(0)}+2k[L(L+1)-\tfrac{1}{4}(k+1)(k-1)]D_{k-2}^{(0)}, \tag{5.47}$$

for the zeroth order, and

$$2(k+1)F^{(0)}D_k^{(n)}=-2(k+1)\sum_{j=1}^{n}F^{(j)}D_k^{(n-j)}-(2k+1)D_{k-1}^{(n)}+(2k+Q+2)\times D_{Q+k}^{(n-1)}+2k[L(L+1)-\tfrac{1}{4}(k+1)\times(k-1)]D_{k-2}^{(n)},\quad n>0. \tag{5.48}$$

From the Hellmann–Feynman theorem,

$$F^{(n+1)}=\frac{1}{n+1}D_Q^{(n)}. \tag{5.49}$$

The computation of the $D_k^{(n)}$ array proceeds columnwise, as before, with the exception that the $k=-1$ row must be calculated separately and included. At the beginning of each perturbation order n, we let $k=0$ in (5.47) and (5.48) to obtain, respectively,

$$D_{-1}^{(0)}=-2F^{(0)},\quad D_{-1}^{(n)}=(Q+2-2/n)D_Q^{(n-1)},\quad n>0. \tag{5.50}$$

The expansion coefficients for $\langle r^{-2}\rangle$ cannot be obtained from (5.47) and (5.48). They can, however, be obtained from an application of the HF theorem, when the angular quantum number L is treated as the parameter in (5.40):

TABLE III. $\langle r^k\rangle$ for the unperturbed hydrogen problem $\hat{H}=-(\hbar^2/2m)\,d^2/dr^2+L(L+1)\hbar^2/2mr^2-b/r$.

k	$\langle r^k\rangle$
3	$\frac{\hbar^6}{8m^3b^3}(35N^6-30N^4L^2-30N^4L+25N^4+3N^2L^4+6N^2L^3-3N^2L^2-6N^2L)$
2	$\frac{\hbar^4}{2m^2b^2}(5N^4-3N^2L^2-3N^2L+N^2)$
1	$\frac{\hbar^2}{2mb}(3N^2-L^2-L)$
0	1
−1	$\frac{mb}{N^2\hbar^2}$
−2	$\frac{2m^2b^2}{\hbar^4(2L+1)N^3}$
−3	$\frac{2m^3b^3}{\hbar^6(2L+1)N^3L(L+1)}$

$$\frac{\partial F}{\partial L}=(2L+1)\langle R^{-2}\rangle. \tag{5.51}$$

From the series expansions in (5.41) and (5.42),

$$D_{-2}^{(n)}=\frac{1}{2L+1}\left(\frac{\partial F^{(n)}}{\partial N}+\frac{\partial F^{(n)}}{\partial L}\right), \tag{5.52}$$

where N has been considered as a function of L. From the unperturbed problem, $N=L+N_R+1$, where N, L, and N_R denote the principal, angular, and radial quantum numbers, respectively. [The term $\partial N/\partial L=1$ has been omitted from (5.52).]

The recursion relations are again easily programmed. [The partial derivatives in (5.52) may be determined by symbolic computation.] There is a major difference, however, between the cases $Q>0$ and $Q<0$. For $Q>0$, the $D_k^{(n)}$ are calculated columnwise first for $k=1,2,3,\ldots$, and then for $k=-1,-2,-3,\ldots$. For $Q<0$, the order is reversed.

For purposes of comparison with the classical problem, the expectation values for several powers of r for the unperturbed hydrogen problem in (5.37) are given in Table III. These are simply the coefficients $C_k^{(0)}$ which are obtained from the $D_k^{(0)}$ by scaling, cf. (5.45). (A significant collection of these values is given in Ref. 53.)

The cases $Q=-1$ and $Q=-2$ in (5.40) represent test cases for which the exact eigenvalue and expectation value expansions can be derived. We omit a discussion of these cases here.

The cases $Q=1$ and $Q=2$, which have been referred to as the Charmonium and Harmonium problems, respectively, have received attention in the context of quark confinement.[54] Expansions to second order for the energy, $\langle r\rangle$ and $\langle r^{-1}\rangle$ for both problems are presented in closed form in Table IV.

The case $Q=-3$ corresponds to the spin-orbit coupling term of the fine structure Hamiltonian.[55] Expansions associated with this problem are also presented in Table IV.

2. Classical perturbed Kepler problems

The Hamiltonian defining the classical Kepler problem has a form similar to the classical hydrogen atom. We wish to consider radial perturbations of the Kepler problem and show that the series expansions may be considered as appropriate classical limits of quantum mechanical series for perturbed hydrogenic atoms.

The problem of two bodies moving under the influence of a potential energy function $V(\mathbf{q})$ which depends only upon their separation can be reduced to a one-body problem in center-of-mass coordinates. The resulting Hamiltonian is given by

$$H=\frac{1}{2m}\left(p_r^2+\frac{p_\theta^2}{r^2}+\frac{p_\phi^2}{r^2\sin^2\theta}\right)+V(r)=\overline{E}^{(0)}, \tag{5.53}$$

where the momenta are defined in terms of their conjugate coordinates as follows:

$$\begin{aligned} p_r&=m\dot{r},\\ p_\theta&=mr^2\dot{\theta},\\ p_\phi&=mr^2\sin^2\theta\dot{\phi}. \end{aligned} \tag{5.54}$$

For the Kepler problem, the potential is given by

$$V(r)=-b/r, \tag{5.55}$$

where $b>0$ is a constant. The action variables for this case are computed to be

$$\begin{aligned} J_\phi&=p_\phi=\text{constant},\\ J_\theta&=\left(p_\theta^2+\frac{p_\phi^2}{\sin^2\theta}\right)^{1/2}-p_\phi=\text{constant},\\ J_r&=-(J_\phi+J_\theta)+b(-m/2\overline{E}^{(0)})^{1/2}. \end{aligned} \tag{5.56}$$

The constants $(p_\theta^2+p_\phi^2/\sin^2\theta)^{1/2}$ and p_ϕ are, respectively, the magnitude of the total angular momentum $\mathbf{L}=\mathbf{r}\times\mathbf{p}$ and its component along the polar axis $\theta=0$. From (5.56), the energy is given by

$$\overline{E}^{(0)}=-\frac{mb^2}{2(J_r+J_\theta+J_\phi)^2}. \tag{5.57}$$

It is convenient to use a canonical transformation to obtain a new set of action variables:

TABLE IV. RSPT series for quantum radially perturbed hydrogen problem with Hamiltonians of the form $\hat{H}=-(\hbar^2/2m)\,d^2/dr^2+L(L+1)\hbar^2/2mr^2-b/r+\lambda r^Q$.

Q=1

$$E=-\frac{mb^2}{2\hbar^2N^2}+\frac{\hbar^2}{2mb}(3N^2-L^2-L)\lambda+\frac{\hbar^6}{8m^3b^4}(-7N^6+3N^2L^4+6N^2L^3+3N^2L^2-5N^4)\lambda^2+\cdots$$

$$\langle r\rangle=\frac{\hbar^2}{2mb}(3N^2-L^2-L)+\frac{\hbar^6}{4m^3b^4}(-7N^6+3N^2L^4+6N^2L^3+3N^2L^2-5N^4)\lambda+\frac{\hbar^{10}}{16m^5b^7}(99N^{10}-21N^6L^4-30N^4L^6-42N^6L^3-90N^4L^5+225N^8$$

$$-21N^6L^2-90N^4L^4-30N^4L^3)\lambda^2+\cdots$$

$$\langle r^{-1}\rangle=\frac{mb}{\hbar^2N^2}+\frac{\hbar^2}{2mb^2}(3N^2-L^2-L)\lambda+\frac{\hbar^6}{2m^3b^5}(-7N^6+3N^2L^4+6N^2L^3+3N^2L^2-5N^4)\lambda^2+\cdots$$

Q=2

$$E=-\frac{mb^2}{2N^2\hbar^2}+\frac{\hbar^4}{2m^2b^2}(5N^4-3N^2L^2-3N^2L+N^2)\lambda+\cdots$$

$$\langle r\rangle=\frac{\hbar^2}{2mb}(3N^2-L^2-L)+\frac{\hbar^8}{8m^4b^5}(-45N^8+14N^6L^2+14N^6L+15N^4L^4+30N^4L^3+25N^4L^2-63N^6+10N^4L)\lambda+\cdots$$

$$\langle r^{-1}\rangle=\frac{mb}{N^2\hbar^2}+\frac{\hbar^4}{m^2b^3}\left(\frac{5N^6-3N^4L^2-3N^4L+N^4}{N^2}\right)\lambda+\cdots$$

Q=−3

$$E=-\frac{mb^2}{2\hbar^2N^2}+\frac{2m^3b^3}{\hbar^6(2L+1)N^3L(L+1)}\lambda+\cdots$$

$$\langle r\rangle=\frac{\hbar^2}{2mb}(3N^2-L^2-L)+\frac{6mN}{\hbar^2(2L+1)L(L+1)}\lambda+\cdots$$

$$\langle r^{-1}\rangle=\frac{mb}{\hbar^2N^2}-\frac{6m^3b^2}{\hbar^6(2L+1)N^3L(L+1)}\lambda+\cdots$$

$$J_1=J_\phi\,,$$

$$J_2=J_\phi+J_\theta\,, \tag{5.58}$$

$$J_3=J_\phi+J_\theta+J_r\,,$$

so that J_2 is the magnitude of the total angular momentum and J_1 is its component along the polar axis. Then

$$\overline{E}^{(0)}(\mathbf{J})=-\frac{mb^2}{2J_3^2}\,. \tag{5.59}$$

This result is seen to represent the classical limit of the quantum term in Eq. (5.38b), where $N\to\infty$, $\hbar\to 0$, $N\hbar=J_3$.

The classical HVHF method will now be used to treat the Kepler problem with a radial perturbation, i.e.,

$$V(r)=-b/r+\lambda r^Q,\quad Q\in\mathbf{Z}. \tag{5.60}$$

The Hamiltonian in (5.53) becomes

$$H=\frac{1}{2m}p_r^2+\frac{J_2^2}{2mr^2}-\frac{b}{r}+\lambda r^Q=\overline{E}(\mathbf{J},\lambda). \tag{5.61}$$

The canonical transformation $P_R=p_r/(2mb)$, $R=2mbr$ yields the scaled Hamiltonian

$$H_{sc}=P_R^2+\frac{J_2^2}{R^2}-\frac{1}{R}+\beta R^Q=\overline{F}(\mathbf{J},\beta), \tag{5.62}$$

where

$$\overline{E}(\mathbf{J},\lambda)=2mb^2\overline{F}(\mathbf{J},\beta),\quad \beta=\frac{\lambda}{b(2mb)^{Q+1}}\,. \tag{5.63}$$

The classical hypervirial relations for the Hamiltonian in (5.61) take the form

$$2(k+1)\overline{F}\,\overline{R^k}=2J_2^2k\overline{R^{k-2}}-(2k+1)\overline{R^{k-1}}$$

$$+\beta(2k+Q+2)\overline{R^{k+Q}}, \tag{5.64}$$

which may be compared to their quantum mechanical counterparts in (5.46).

The expectation values for several powers of r for the unperturbed Kepler problem, $\lambda=0$ in Eq. (5.61), are given in Table V. A comparison with the corresponding

TABLE V. $\overline{r^k}$ for the Kepler hydrogen problem $H=(1/2m)\,p_r^2+J_2^2/2mr^2-b/r$.

k	$\overline{r^k}$
3	$\frac{1}{8m^3b^3}(35J_3^6-30J_3^4J_2^2+3J_3^2J_2^4)$
2	$\frac{1}{2m^2b^2}(5J_3^4-3J_3^2J_2^2)$
1	$\frac{3J_3^2-J_2^2}{2mb}$
0	1
−1	$\frac{mb}{J_3^2}$
−2	$\frac{m^2b^2}{J_2J_3^3}$
−3	$\frac{m^3b^3}{J_2^3J_3^3}$

quantum values in Table III shows that the classical values are obtained in the limit

$$N\to\infty,\ L\to\infty,\ \hbar\to 0,\ \text{such that } N\hbar=J_3,\ L\hbar=J_2. \tag{5.65}$$

Expansions for the cases $Q=1$, 2 and -3 are shown in Table VI. These series may be compared to the quantum series in Table IV. The classical limit in (5.65) is seen to hold.

The $Q=-3$ perturbation in (5.61) is of interest because it represents a relativistic correction to the Kepler problem (Ref. 1, p. 511). In addition, it represents the first correction in the problem of an orbit of a satellite about an oblate planet without air drag.[56] Brouwer[57] used the Poincaré–von Zeipel method to obtain the energy series to second order; Kozai[58] extended this series to third order. The classical HVHF method may be easily used to generate the series to higher order, either algebraically or numerically.

TABLE VI. Canonical perturbation series for classical radially perturbed Kepler problem with Hamiltonians of the form $H=p_r^2/2m+J_2^2/r^2-b/r+\lambda r^Q=E$.

Q=1

$$\overline{E}=-\frac{mb^2}{2J_3^2}+\frac{3J_3^2-J_2^2}{2mb}\lambda+\frac{-7J_3^6+3J_3^2J_2^4}{8m^3b^4}\lambda^2+\cdots$$

$$\overline{r}=\frac{3J_3^2-J_2^2}{2mb}+\frac{-7J_3^6+3J_3^2J_2^4}{4m^3b^4}\lambda+\frac{99J_3^{10}-21J_3^6J_2^4-30J_3^4J_2^6}{16m^5b^7}\lambda^2+\cdots$$

$$\overline{r^{-1}}=\frac{mb}{J_3^2}+\frac{3J_3^2-J_2^2}{2mb^2}\lambda+\frac{-7J_3^6+3J_3^2J_2^4}{2b^5m^3}\lambda^2+\cdots$$

Q=2

$$\overline{E}=-\frac{mb^2}{2J_3^2}+\frac{1}{2m^2b^2}(5J_3^4-3J_2^2J_3^2)\lambda$$
$$+\frac{1}{16m^3b^6}(-143J_3^{10}+90J_3^8J_2^2+21J_3^6J_2^4)\lambda^2+\cdots$$

$$\overline{r}=\frac{1}{2mb}(3J_3^2-J_2^2)+\frac{-45J_3^8+14J_3^6J_2^2+15J_3^4J_2^4}{8m^4b^5}\lambda+\cdots$$

$$\overline{r^{-1}}=\frac{mb}{J_3^2}+\frac{5J_3^6-3J_3^4J_2^2}{m^2b^3J_3^2}\lambda+\cdots$$

Q=−3

$$\overline{E}=-\frac{mb^2}{2J_3^2}+\frac{m^3b^3}{J_2^2J_3^2}\lambda+\frac{m^5b^4(-6J_3J_2-15J_3^2+3J_2^2)}{4J_3^5J_2^2}\lambda^2+\cdots$$

$$\overline{r}=\frac{3J_3^2-J_2^2}{2mb}+\frac{3mJ_3}{J_2^2}\lambda-\frac{3m^3b(15J_3^4-2J_2J_3^2-J_2^4)}{4J_2^2J_3^3}\lambda^2+\cdots$$

$$\overline{r^{-1}}=\frac{mb}{J_3^2}-\frac{3m^3b^2}{J_2^2J_3^3}\lambda+\frac{m^5b^3(6J_2J_3+15J_3^2-3J_2^2)}{J_2^2J_3^5}\lambda^2+\cdots$$

VI. CONCLUDING REMARKS

The classical hypervirial and Hellmann–Feynman theorems have been shown to provide a powerful method of generating canonical perturbation expansions for separable Hamiltonians. As in the quantum mechanical version, where there is no need to calculate wave functions, the classical method bypasses the tedious requirement to calculate the Fourier series expansions for the generating functions. There are some other interesting systems which could be explored with this method, e.g., the Stark effect in hydrogen (the quantum mechanical HVHF version was studied by Austin[52]). Apart from these purely computational aspects, however, is the correspondence between quantum and classical HV and HF theorems which describe eigenstates and periodic orbits, respectively. This correspondence is provided by the action-preserving classical limit discussed by Turchetti,[14] Graffi and Paul,[15] and others.

For the more general nonseparable problems, however, the most effective route to generate classical expansions may still be to take the classical limit of quantum Rayleigh–Schrödinger perturbation expansions.

ACKNOWLEDGMENTS

The authors are grateful for the support provided by the Natural Sciences and Engineering Research Council of Canada (NSERC) in the form of a Postgraduate Scholarship (SMM) and an Operating Grant in Aid of Research (ERV).

APPENDIX: RELATION BETWEEN CANONICAL AND NONCANONICAL PERTURBATION METHODS

A variety of perturbation methods for differential equations (nonlinear oscillations) may also be used to

study the classical problems mentioned in Sec. II A. However, in contrast to the perturbation theory outlined in that section, these methods are generally not canonical: the transformations associated with these methods (i.e., change of variables, scaling of coordinates) are not necessarily subject to the strict rules of canonical transformations. Since this aspect of perturbation theory is rarely addressed in the literature, it is worthwhile to consider an illustrative example and to show how the canonical and noncanonical methods can be related.

Our example will be the quartic anharmonic oscillator Hamiltonian, $M=4$ in (2.12). In this case, Hamilton's equations lead to the Duffing equation:

$$\ddot{x}+\omega_0^2 x+\epsilon x^3=0, \tag{A1}$$

where $\epsilon=4\lambda/m$. In (one version of) the Poincaré–Linstedt method of strained parameters,[59] a series solution of the form

$$x(t)=x_0(t)+\epsilon x_1(t)+\epsilon^2 x_2(t)+\cdots \tag{A2}$$

is assumed along with a scaling of the time variable (in order to remove *secular terms*),

$$s=\omega t=(\omega_0+\epsilon\omega_1+\epsilon^2\omega_2+\cdots)t. \tag{A3}$$

Substitution of Eqs. (A2) and (A3) into Eq. (A1) and collection of terms in ϵ^n, $n=0,1,2,\ldots$ leads to a hierarchy of second-linear differential equations, beginning with the unperturbed problem,

$$x''_0(s)+x_0(s)=0, \quad x_0(0)=c_1, \quad x''_0(0)=c_2, \tag{A4}$$

where the primes indicate differentiation with respect to s, followed by the general nth order problem,

$$x''_n(s)+x_n(s)=f_n(s), \tag{A5}$$

where the inhomogeneous term $f_n(s)$ is determined by $x_0(s),\ldots,x_{n-1}(s)$ and their derivatives. A knowledge of solutions $x_0\cdots x_n$ permits the calculation of x_{n+1}. At each order n, the removal of secular terms leads to the determination of the coefficient ω_n in Eq. (A3). The net result is

$$x(t)=a\cos(\omega t+\phi)+\frac{\epsilon a^3}{32\omega_0^2}\cos 3(\omega t+\phi)+\frac{\epsilon^2 a^5}{1024\omega_0^4}\times[-21\cos 3(\omega t+\phi)+\cos 5(\omega t+\phi)]+\cdots, \tag{A6}$$

where a and ϕ are determined by the initial conditions and the frequency $\omega=\omega(\epsilon)$ is given by the series expansion

$$\omega(\epsilon)=\omega_0\left(1+\frac{3a^2\epsilon}{8\omega_0^2}-\frac{15a^4\epsilon^2}{256\omega_0^4}+\cdots\right). \tag{A7}$$

Note that the solution $x(t)$ is periodic with period $T=2\pi/\omega$. As well, its amplitude may be written explicitly as a function $A(a,\epsilon)$, where $A(a,0)=a$.

The action associated with the periodic solution $x(t)$ in Eq. (A6) may be computed by the relation

$$J=\frac{1}{2\pi}\oint p\,dx=\frac{m}{2\pi}\int_0^T \dot{x}^2\,dt. \tag{A8}$$

After some algebra, we find

$$J(a,\lambda)=\frac{m\omega_0 a^2}{2}+\frac{3a^4}{4\omega_0}\lambda-\frac{51a^6}{128m\omega_0^3}\lambda^2+\cdots. \tag{A9}$$

It is seen that the perturbation method produces solutions whose classical actions do not remain unchanged with λ. The energy associated with the periodic solution $x(t)$ may be found by substitution into the Hamiltonian in (2.12). To second order in λ

$$\bar{E}(a,\lambda)=\frac{m\omega_0^2 a^2}{2}+\frac{9a^4}{8}\lambda+\frac{25a^6}{128m\omega_0^2}\lambda^2+\cdots. \tag{A10}$$

As it stands, this "noncanonical" series bears no obvious resemblance to the canonical series in Eq. (2.18b), which corresponds to fixed action J. However, it can be recovered from the canonical series by allowing J to vary with λ as given in Eq. (A9): substituting the series in Eq. (A9) into the canonical series Eq. (2.18b) does, in fact, yield Eq. (A10).

It has also been shown[60,61] that the first-order contributions to these noncanonical perturbation expansions can be obtained by a classical limit of the quantum mechanical perturbation series associated with perturbed coherent states. The classical limit, although involving $\hbar\to 0$, is noncanonical, since it does not preserve the action. Some further studies in this direction have been made:[62] second-order contributions to the frequency expansions may be retrieved but the method breaks down beyond this correction.

[1] H. Goldstein, *Classical Mechanics* (Addison–Wesley, Reading, MA, 1980), 2nd ed.
[2] E. J. Saletan and A. H. Cromer, *Theoretical Mechanics* (Wiley, New York, 1971).
[3] A. J. Lichtenberg and M. A. Lieberman, *Regular and Stochastic Motion* (Springer, New York, 1983).
[4] G. Gallavotti, *The Elements of Mechanics* (Springer, New York, 1983).
[5] J. O. Hirshfelder, J. Chem. Phys. **33**, 1462 (1960).
[6] (a) H. Hellmann, *Einführung in die Quantenchemie* (Deuticke, Vienna, 1937); (b) R. P. Feynman, Phys. Rev. **56**, 340 (1939).
[7] R. J. Swenson and S. H. Danforth, J. Chem. Phys. **57**, 1734 (1972).
[8] J. Killingbeck, Phys. Lett. A **65**, 87 (1978).
[9] J. O. Hirschfelder, Z. Phys. Chem. (Neue Folge) **37**, 167 (1963).

[10] W. A. McKinley, Am. J. Phys. **39**, 905 (1971).
[11] G. D. Birkhoff, *Dynamical Systems* (American Mathematical Society, New York, 1927), Vol. IX.
[12] F. G. Gustavson, Astron. J. **71**, 670 (1966).
[13] J. R. Cary, Phys. Rep. **79**, 129 (1981).
[14] G. Turchetti, Nuovo Cimento B **82**, 203 (1984).
[15] S. Graffi and T. Paul, Comm. Math. Phys. **108**, 25 (1987).
[16] G. Alvarez, S. Graffi, and H. J. Silverstone, Phys. Rev. A **38**, 1687 (1988).
[17] G. Alvarez, J. Phys. A **22**, 617 (1989).
[18] R. T. Swimm and J. B. Delos, J. Chem. Phys. **71**, 1706 (1979).
[19] W. P. Reinhardt and C. Jaffe, in *Quantum Mechanics in Mathematics, Chemistry and Physics*, edited by K. E. Gustafson (Plenum, New York, 1981), p. 167; C. Jaffe and W. P. Reinhardt, J. Chem. Phys. **77**, 5191 (1982); R. B. Shirts and W. P. Reinhardt, J. Chem. Phys. **77**, 5204 (1982); W. P. Reinhardt and D. Farelly, J. Phys. (Colloque) **43**, C2 (1982); W. P. Reinhardt, in *Mathematical Analysis of Physical Systems*, edited by R. E. Mickens (Van Nostrand, New York, 1985), p. 169.
[20] M. Robnik, J. Phys. A: Math. Gen. **17**, 109 (1984).
[21] W. R. Wood and M. K. Ali, J. Phys. A: Math. Gen. **20**, 351 (1987).
[22] M. K. Ali, J. Math. Phys. **26**, 2565 (1985).
[23] B. Eckhardt, J. Phys. A: Math. Gen. **19**, 2961 (1986).
[24] (a) M. K. Ali, W. R. Wood, and J. S. Devitt, J. Math. Phys. **27**, 1806 (1986); (b) M. K. Ali and W. R. Wood, Prog. Theor. Phys. **78**, 766 (1987); (c) M. K. Ali and W. R. Wood, J. Math. Phys. **30**, 1238 (1989).
[25] B. W. Char, K. O. Geddes, G. H. Gonnet, M. B. Monagan, and S. M. Watt, *MAPLE Reference Manual* (WATCOM Publications, Waterloo, 1988), 5th ed.
[26] C. Lanczos, *The Variational Principles of Mechanics* (Dover Publications, New York, 1970), 4th ed.
[27] M. W. Hirsch and S. Smale, *Differential Equations, Dynamical Systems, and Linear Algebra* (Academic, New York, 1974).
[28] J. Guckenheimer and P. Holmes, *Nonlinear Oscillations, Dynamical Systems and Bifurcations of Vector Fields* (Springer, New York, 1983).
[29] J. O. Hirschfelder, W. Byers Brown, and S. T. Epstein, Adv. Quant. Chem. **1**, 225 (1964).
[30] C. M. Bender and T. T. Wu, Phys. Rev. Lett. **27**, 461 (1971).
[31] E. R. Vrscay, Phys. Rev. Lett. **53**, 2521 (1984).
[32] B. Simon, Ann. Phys. (NY) **58**, 76 (1970).
[33] J. H. Epstein and S. T. Epstein, Am. J. Phys. **30**, 266 (1962).
[34] G. Marc and W. G. McMillan, Adv. Chem. Phys. **58**, 209 (1985).
[35] F. M. Fernandez and E. A. Castro, *Hypervirial Theorems*, Lecture Notes in Chemistry, Vol. 43 (Springer, New York, 1987).
[36] F. M. Fernandez and E. A. Castro, Phys. Rev. A **24**, 2344 (1981); Int. J. Quant. Chem. **19**, 521 (1981); **19**, 533 (1981).
[37] J. I. Musher, Am. J. Phys. **34**, 267 (1966).
[38] W. Pauli, *Handbuch der Physik* (Springer, Berlin, 1933).
[39] N. Bleistein and R. A. Handelsman, *Asymptotic Expansions of Integrals* (Dover, New York, 1986).
[40] E. P. Wigner, Phys. Rev. **40**, 749 (1932); see also M. Hillery, R. F. O'Connell, M. O. Scully, and E. P. Wigner, Phys. Rep. **106**, 121 (1984).
[41] M. V. Berry, Trans. R. Soc. London, Ser. A **287**, 237 (1977).
[42] J. Killingbeck, J. Phys. A: Math. Gen. **20**, 601 (1987).
[43] S. Graffi and V. Grecchi, J. Math. Phys. **19**, 1002 (1978).
[44] E. Caliceti, S. Graffi, and M. Maioli, Commun. Math. Phys. **75**, 51 (1980).
[45] W. B. Jones and W. J. Thron, *Continued Fractions, Analytic Theory and Applications* (Addison-Wesley, Reading, MA, 1980).
[46] P. Henrici, *Applied and Computational Complex Analysis* (Wiley, New York, 1977), Vol 2.
[47] E. R. Vrscay and J. Cizek, J. Math. Phys. **27**, 185 (1986).
[48] E. R. Vrscay, J. Math. Phys. **29**, 901 (1988).
[49] G. A. Baker, *Essentials of Padé Approximants* (Academic, New York, 1975).
[50] J. D. Louck and H. W. Galbraith, Rev. Mod. Phys. **48**, 69 (1976).
[51] M. Grant and C. S. Lai, Phys. Rev. A **20**, 718 (1979).
[52] E. J. Austin, Mol. Phys. **40**, 893 (1980); **42**, 1391 (1981).
[53] H. A. Bethe and E. E. Salpeter, *Quantum Mechanics of One- and Two-Electron Atoms* (Springer, Berlin, 1957).
[54] C. Quigg and J. L. Rosner, Phys. Rep. **56**, 167 (1979).
[55] C. Cohen-Tannoudji, B. Diu, and F. Laloë, *Quantum Mechanics* (Wiley, New York, 1977), Vol. 2.
[56] A. E. Roy, *Orbital Motion* (Adam Hilger, Bristol, 1988).
[57] D. Brouwer, Astron. J. **64**, 378 (1959).
[58] Y. Kozai, Astron. J. **67**, 446 (1962).
[59] A. H. Nayfeh, *Perturbation Methods* (Wiley, New York, 1973).
[60] K. Bhaumik and B. Dutta-Roy, J. Math. Phys. **16**, 1131 (1975); R. Dutt and M. Lakshmanan, J. Math. Phys. **17**, 482 (1976).
[61] S. K. Bose and U. B. Dubey, Fortsch. Phys. **35**, 675 (1987).
[62] P. M. Benoit, S. M. McRae, and E. R. Vrscay (in preparation).