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Action-Variable Theory and Classical Frequencies*

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A Hamilton–Jacobi/action–angle variable perturbation theory for the calculation of the frequency of oscillation of a classical system which undergoes periodic motion is developed and illustrated. The theory is based upon a contour integral definition of the action variable plus a particular expansion of the momentum function which is the integrand of the contour integral. The basic result of the theory is a series representation for the action variable which is easy to use and powerful. Analytic and numerical examples of the application of the action-variable/frequency formalism are given.

I. INTRODUCTION/CONCLUSIONS

For a classical system in which periodic motion occurs the frequency of oscillation is a quantity of fundamental interest. Oscillatory motion occurs in, e.g., numerous mechanical, electromagnetic, electronic, and acoustical systems. The frequency appears also as a critical ingredient in the interaction between two systems; an example is the significance of the frequency in the electromagnetic radiation from an oscillating electric charge. For a system undergoing periodic motion a knowledge of the frequency of oscillation is often sufficient. Thus, techniques for the direct calculation of the frequency of a classical system are of interest.

One method to obtain the frequency of a periodic system is to solve the equation of motion. Besides the straightforward numerical integration of the dynamical equation, various perturbative techniques exist for solving the dynamical equation for systems whose motions consist of a well-understood motion, such as simple-harmonic or coulombic motion, plus a "smaller" motion due to a "perturbative" term in the dynamical equation [1–3]. While these perturbative techniques are usually easy to apply in low order, they may be difficult to use in high order. More importantly, however, is that it is conceptually and practically inefficient to obtain the

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complete system motion just to obtain the frequency of oscillation. Thus, a direct method of obtaining the frequency is useful.

As is well known, the action variable in classical Hamilton–Jacobi theory provides a direct means of obtaining the frequency of oscillation of a system undergoing periodic motion. Hamilton–Jacobi theory, which itself is a part of canonical transformation theory, provides a method for the complete solution of dynamical problems [4, 5]. However, in the specific form of Hamilton–Jacobi theory known as the theory of action–angle variables [4–6], the action variable can be used to find the system frequency without recourse to the rest of the theory.

It would appear that calculating the action variable is the obvious method for obtaining the frequency of a periodic classical system. However, the action variable is an integral of the momentum function over one cycle of the motion, and the integral may not be done easily. While an action-variable integral can always be done numerically, such a procedure does not result in an analytic form, and, further, tends to obscure the physics. What is needed is a technique which allows ready computation of the action variable, and, in addition, permits the basic physics of the action variable to be seen.

The basis for the calculation of frequencies via the action variable presented in this paper is a contour integral definition of the action variable combined with a particular expansion of the momentum function which is the integrand of the contour integral. The expansion of the momentum function is a Laurent expansion, which means that the action variable is just the coefficient of the first inverse power in the expansion [7, 8]. Thus, expanding the momentum functon does the action-variable integral automatically.

The formalism presented here we call action-variable perturbation theory (AVPT). For certain systems, such as the harmonic oscillator, the action variable is a simple analytic function of the energy. In most cases, however, the action variable cannot be found in closed form; in these instances the AVPT enables one to obtain a representation of the action variable as an expansion in powers of an appropriate parameter characterizing the system. Because of the series representation of the action variable we call the formalism a perturbation theory; however, as will be seen below, the formalism is more general than the usual perturbation theories.

We are now in a position to make a series of observations and conclusions about the action-variable perturbation theory. First, the AVPT series representation of the action variable contains the expansion parameter in the coefficients as well as in the powers. The consequence of this is that the series is more powerful than the usual perturbation series. Second, one or several terms of the AVPT series is usually sufficient to solve accurately most problems. This means that simple closed expressions of the action variable and frequency are easily obtained. Third, the AVPT applies to all systems, not just to those systems which consist of an exactly solvable hamiltonian plus a perturbing potential. The theory does not require the solution of an unperturbed problem. Fourth, the formalism provides a theoretical framework in which all orders and all potentials are treated by one procedure. Being based on the theory of action–angle variables, however, the theory applies only to separable

systems. Fifth, AVPT is exceptionally fast on a computer, and gives good or high accuracy. Sixth, the action-variable formalism provides an alternate interpretation of the energy structure (dependence) of classical frequencies. The frequency is seen as arising from singularities of the momentum function in the complex coordinate plane.

The above remarks and conclusions are illustrated in the following sections. Lastly, we remark that the definition of the classical action variable as a contour integral in the complex coordinate plane is the starting point of a theory of action–angle variables in quantum mechanics [9, 10]. Also, the classical perturbation theory presented here is closely related to a corresponding quantum perturbation theory [11].

II. Action-Variable Formalism

The classical action-variable perturbation theory is founded upon the action variable $J(E)$ [4–6]. We are interested in the frequency of a particle moving in one dimension x in a potential well $V(x)$. The particle has energy E and mass m such that $2m=1$. We define $J(E)$ as a contour integral of the momentum function $p(x, E)$:

$$J(E)=\frac{1}{2\pi}\int_C dx\, p(x, E). \tag{1}$$

The momentum function is defined as

$$p(x, E)=[E-V(x)]^{1/2} \tag{2}$$

where the square root is specified on the complex x plane as follows. The periodic motion occurs between the two physical turning points x_1, x_2 defined by $p(x_1, E)=p(x_2, E)=0$. The complex x plane on which $p(x, E)$ is defined is given a cut from x_1 to x_2 along the real x axis. The square root in (2) is that branch of the function which is positive just below the cut. Returning to the action variable (1), the contour C is defined as enclosing counterclockwise the two turning points and the section of real x axis between them. An illustration of the cut x plane and contour C is given in Fig. 1a.

AVPT is based upon a series representation for the action variable (1). Since $J(E)$ contains $p(x, E)$, an effective series for $p(x, E)$ is sought. As $p(x, E)$ vanishes at the turning points x_2 and x_1 $(=-x_2)$, a useful standard form of $p(x, E)$ is

$$p(x, E)=[-Ex_2^{-2}(x^2-x_2^2)]^{1/2}f(x) \tag{3}$$

where $f(x)$ is dimensionless and obeys $f(0)=1$. (The discussion is restricted, for the moment, to potentials for which $V(0)=0$ and $V(x)=V(-x)$.) The factors in $p(x, E)$ are expanded. Since the contour C used in (1) occurs in the region $|x|>x_2$,

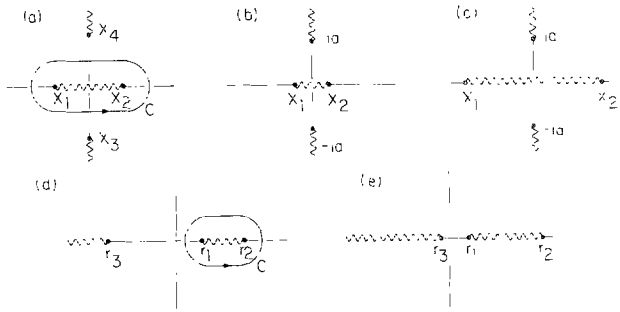

FIG. 1 (a) The complex x plane on which the momentum function $p(x, E)$ is defined for the anharmonic oscillator. x_1 and x_2 are the physical turning points. A cut (zigzag line) runs between x_1 and x_2, and the contour C used in defining the action variable $J(E)$ encloses x_1 and x_2 and the cut (see Eq (1)). The unphysical turning points x_3 and x_4 are on the imaginary x axis. Additional cuts begin on x_3 and x_4. (b) and (c) The complex x plane for $p(x, E)$ for the resonance well $V(x) = -V_0/(x^2 + a^2)$. $p(x, E)$ has four branch points, the turning points x_1 and x_2, and $\pm ia$. (b) For energy E near the bottom of the well $x_2 < a$ and $-\alpha < 1$ (see text). (c) For E near the top of the well $x_2 > a$ and $-\alpha > 1$. (d) and (e) The complex r plane on which $p(r, E, L)$ is defined for the three-dimensional radial system with effective potential $-g/r + \lambda r + L^2/r^2$. Contour C encloses the physical turning points r_1 and r_2 and the cut between them. (d) For E near the bottom of the well $r_2 < -r_3$ and $-\alpha < 1$ (see text). (e) For E significantly above the bottom of the well $r_2 > -r_3$ and $-\alpha > 1$.

the factor $(x^2 - x_2^2)^{1/2}$ is expanded in the form $x(1 - x_2^2/x^2)^{1/2} = x \sum c(k)(x_2^2/x^2)^k$, where $k = 0, 1, 2, \ldots$, $c(k)$ is the square root expansion coefficient, and $|x| > x_2$. $f(x)$ is expanded in the form

$$f(x) = \sum_{k=0}^{\infty} u(k)\, \alpha^k (x^2/x_2^2)^k \tag{4}$$

where $u(0) = 1$. α is a dimensionless expansion parameter which occurs in the series for $J(E)$ (see below). The expansion of $f(x)$ is valid in the region $|x| < |x_s|$, where x_s is the location of the nearest singularity of $f(x)$. Using the $(x^2 - x_2^2)^{1/2}$ and $f(x)$ expansions in the standard form (3) yields the desired expansion of $p(x, E)$:

$$\begin{aligned} p(x, E) &= i \sum_{r=0}^{\infty} \sum_{n=-r}^{\infty} b(n, r)\, \alpha^r x^{1-2n}, \\ b(n, r) &= \sqrt{E}\, x_2^{2n-1}\, c(n + r)\, u(r). \end{aligned} \tag{5}$$

Expansion (5) is valid in the region $x_2 < |x| < |x_s|$. Note that $b(n, r) = 0$ for $n + r < 0$ or $r < 0$.

The perturbation series representation for $J(E)$ follows immediately from (5) either by using Laurent's theorem or by substituting (5) into (1) and using the residue theorem:

$$J_N(E) = -\sum_{r=0}^{N} b(1, r)\, \alpha^r. \tag{6}$$

Equation (6) is a series representation for $J(E)$ to order N in the parameter α. As will be seen in the illustrations, (6) may be convergent or divergent; in either case it provides a powerful method for finding $J(E)$ and the system frequency.

Before showing ways that (6) can be used and discussing its physical content, we note that to use (6) it is necessary to obtain the turning point x_2 and the $f(x)$ expansion coefficients $u(k)$. x_2 and $u(k)$ are key ingredients in (5) and thus also in (6).

As the frequency $v(E)$ of oscillation of the particle in the potential well is related to the action variable $J(E)$ by $1/v = 2\pi\, \partial J/\partial E$, a series representation for $1/v$ follows immediately from (6):

$$\begin{aligned} 1/v(E) &= -\sum_{r=0}^{N} g(r)\,\alpha^r, \\ g(r) &= 2\pi\left[\frac{\partial b(1,r)}{\partial E} + b(1,r)\,\frac{r}{\alpha}\,\frac{\partial \alpha}{\partial E}\right]. \end{aligned} \tag{7}$$

To obtain $v(E)$ one can use either (6) and differentiate, or (7). In the following we emphasize the use of (6).

Although it is easy to generate (6) or (7) to any order N, the lower orders are instructive and are frequently highly accurate. Order zero is obtained from (6) with $N=0$ and the properties of $c(k)$ and $u(k)$:

$$J_0(E) = \tfrac{1}{2}\sqrt{E}\,x_2(E). \tag{8}$$

Order zero means approximating $p(x, E)$ by $[p(x, E)]^2 = -Ex_2^{-2}(x^2 - x_2^2) = E - (E/x_2^2)\,x^2$. Thus, in this order, $p(x, E)$ represents a harmonic oscillator with turning points x_2 and x_1 $(= -x_2)$. That is, in lowest order, formulae (5)–(7) mean that the potential $V(x)$ has been approximated by an oscillator well $(E/x_2^2)\,x^2$ whose turning points are the same as the exact physical turning points x_1 and x_2. In this order the system frequency is $1/v = 2\pi\partial J_0/\partial E$.

Orders one $(N=1)$ and two $(N=2)$ follow similarly from (6), (5), (8) and the properties of $c(k)$ and $u(k)$:

$$J_1(E) = J_0(E)[1 + u(1)\,\alpha/4], \tag{9}$$

$$J_2(E) = J_0(E)[1 + u(1)\,\alpha/4 + u(2)\,\alpha^2/8]. \tag{10}$$

In the expansion of $f(x)$ the combination $u(k)\,\alpha^k$ occurs so that the separation between $u(k)$ and α^k is arbitrary. However, as will be seen in the illustrations, each system has a natural, physical choice for the definition of α. Further, α is frequently small. Thus, in (9) and (10), e.g., the $u(1)\alpha$ and $u(2)\alpha^2$ terms are seen as corrections on the zeroth order form $J_0(E)$. Lastly, as $x_2(E)$, $\alpha(E)$, $u(1)$ and $u(2)$ are easily calculated, even by hand, (8)–(10) are useful expressions for obtaining $J(E)$ and the system frequency.

As will be seen in the illustrations and as was mentioned above, series (6) for $J(E)$ can be divergent. Various techniques exist for summing divergent series [12]; the one we employ here is the Shanks transformation [12, 13]. For order two the Shanks transformation estimate for $J(E)$ is

$$J_{2S}=\frac{J_2J_0-J_1^2}{J_2+J_1-2J_1}. \tag{11}$$

Use of (8)–(10) in (11) gives, e.g.,

$$J_{2S}=J_0\left[1+\frac{(u(1)\,\alpha)^2/4}{u(1)\,\alpha-u(2)\,\alpha^2/2}\right]. \tag{12}$$

Although simple, (12) is a powerful representation of $J(E)$.

An overview of the calculational techniques is: For smaller α, (8)–(10) are simple to use and accurate. Equation (8) by itself is frequently excellent. For larger α, (12) is simple and effective. For very large α or very high accuracy, (6) is used with $N\geqslant 3$. For $N\geqslant 3$ the series (6) can be used with or without the Shanks transformation.

As mentioned above in the discussion of the low order forms J_0, J_1, and J_2, an interpretation of the basic equations (1) (6) is that in zeroth order they represent the embedding of a particular oscillator in the system defined by $V(x)$; the action variable for this special oscillator is $J_0(E)$. Corrections to order zero are provided then by the higher order terms in (6). This point of view can be emphasized by rewriting (6) as

$$J_N(E)=J_0(E)\sum_{r=0}^{N}\bar{b}(1,r)\,\alpha^r \tag{13}$$

with $\bar{b}(1,r)=b(1,r)/b(1,0)$ and $\bar{b}(1,0)=1$. In the form (13) one sees the series as "correcting," to order N in α, the embedded oscillator form $J_0(E)$.

A second interpretation of (1)–(6) follows from an examination of the meaning of (5) and how it is used in (1) to produce (6). In addition to the cut from x_1 to x_2 along the real x axis, the momentum function $p(x, E)$ will have in general other singularities (see Fig. 1). When the contour C in (1) is distorted to enclose the point at infinity it will pick up contributions from these singularities; in fact, one may say that these singularities determine $J(E)$ and thus also the system frequency $\nu(E)$. The meaning of (5) and (6) can now be seen as follows. Because of the residue theorem, the only term in the double series (5) that contributes to the $J(E)$ integral (1) is the x^{-1} term. Thus, for purposes of use in (1) only, we may write $p(x, E)$ as

$$p(x,E)=\frac{i}{x}\sum_{r=0}^{\infty}b(1,r)\,\alpha^r. \tag{14}$$

But the form (14) is just the $p(x, E)$ of a pure oscillator with residue $i\sum b(1,r)\,\alpha^r$ in

the neighborhood of infinity. Thus, we see that the impact of expansion (5) is to sweep the effects of the singularities of $p(x, E)$ into the point $x=\infty$ by including their effects in the residue of the x^{-1} term in $p(x, E)$. In other words, expansion (5) has the effect of making a non-harmonic oscillator into a pure-harmonic oscillator with the correct frequency.

The basic equations of the AVPT, (1)–(6), are founded upon the analytic properties of $f(x)$, $p(x, E)$, and $V(x)$. In particular, implicit in the development of (1)–(6) is the assumption of an analytic form for $V(x)$, and the potentials used to illustrate (1)–(6) in the following sections are all of this type. Although it is outside the domain of the present discussion, one can ask if (1)–(6) apply to potentials which are specified, e.g., numerically and so are not defined by an analytic form. For such a "numerical" potential one could proceed as follows. As mentioned shortly after (6), the key elements of (5) and thus of (6) are x_2 and $u(k)$. Given a numerical $V(x)$ one can determine a numerical x_2 and $f(x)$ from (3), and then, having $f(x)$, find the $u(k)$ from (4) using one of the standard numerical methods. In this way the program of (1)–(6) can be carried out numerically. While this numerical procedure is satisfactory, it does not illustrate the kind of system (1)–(6) is designed for, and we do not consider it further here.

III. Anharmonic Oscillators

Our first illustration of the use of the AVPT is the anharmonic oscillator. To begin, we take the potential to be $V(x)=(1-\lambda)x^2+\lambda x^4$ so that $\lambda=0$ is a pure harmonic oscillator and $\lambda=1$ is a pure anharmonic oscillator. The momentum function is $p(x, E)=[E-(1-\lambda)x^2-\lambda x^4]^{1/2}$ and the system has four turning points $-x_1=x_2=[(\mu-\lambda_1)/2\lambda]^{1/2}$ and $-x_3=x_4=i[(\mu+\lambda_1)/2\lambda]^{1/2}$ where $\lambda_1=1-\lambda$ and $\mu=(\lambda_1^2+4\lambda E)^{1/2}$. x_1 and x_2 are the physical turning points, while x_3 and x_4 are unphysical. A picture of the cut x plane for the anharmonic oscillator $p(x, E)$ is shown in Fig. 1a; the cuts begin on the turning points. Next, using the standard form (3) for $p(x, E)$ one finds $f(x)=(1-x^2/x_4^2)^{1/2}$, and, by expanding, $f(x)=(1-\alpha x^2/x_2^2)^{1/2}=\sum c(k)\,\alpha^k(x^2/x_2^2)^k$, where $c(k)$ is the square root expansion coefficient, $k=0, 1, 2,...$, and the choice $\alpha=x_2^2/x_4^2$ arises naturally. Comparing the above expansion of $f(x)$ with the standard expansion (4) gives $u(k)=c(k)$. The definitions of x_2, x_4, α, and $u(k)$ used in (5), (6) gives the solution of the anharmonic oscillator. (We note that expansion (5) for the anharmonic oscillator case is a generalization of a series due to Boguslawski [14].)

Before showing a numerical test of the anharmonic oscillator solution, it is useful to examine the validity of the expansions in (5), (6) for this case. x_3 and x_4 are the first (and only) singularities of $p(x, E)$ that one encounters outside of the contour C (see Fig. 1a). Thus, (5) is valid in $x_2<|x|<|x_4|$ which is a ring of inner radius x_2 and outer radius $|x_4|$. Inspection of the x_2, x_4 formulae shows that $x_2\leqslant|x_4|$ so that the ring of validity of (5) has a finite width. For $\lambda=1$, $x_2=|x_4|$, and the ring

becomes vanishingly thin; (5) and (6) are still useful, however, as will be seen below. The expansion parameter α is x_2^2/x_4^2. For $\lambda \simeq 0$, $\alpha \simeq -\lambda E$, while as $\lambda \to 1$, $\alpha \to -1$. Thus, as expected from the discussion of Section II, the expansion parameter is small for the mostly harmonic cases ($\lambda \simeq 0$) and large for the mostly anharmonic cases ($\lambda \simeq 1$).

The numerical results of (1)–(6) for the anharmonic oscillator are shown in Fig. 2a for the energy $E = 1.0$ and the four λ values 0.001, 0.1, 0.3, and 1.0. As a measure of the effectiveness of (6) we define the accuracy A_N for a given order N by

$$A_N = \left| \frac{J_N(E) - J_R(E)}{J_R(E)} \right| \tag{15}$$

where J_N is given by (6) and J_R is a reference value for J. The reference value J_R is obtained by numerical integration and is accurate to one part in 10^9 or better; we have not tried to exceed this level of accuracy in this paper although (6) can do better than this under many conditions. Turning now to Fig. 2a, we see that for $\lambda = 0.001$ the accuracy of (6) is a part in 10^4 for order zero and a part in 10^8 for order one. For $\lambda = 0.1$, zeroth order is good to one percent, while first and second order give good accuracy, and the accuracy improves rapidly with order N. Similar behavior obtains for $\lambda = 0.3$. For $\lambda = 1.0$, the pure anharmonic case, the accuracy is 10% in order zero, one percent in order one, and improves slowly with order N reaching one part in 10^4 in order eight.

We make three comments on the data of Fig. 2a. First, as expected on the basis of our earlier discussion, series (6) for $J_N(E)$ is most effective for the nearly har-

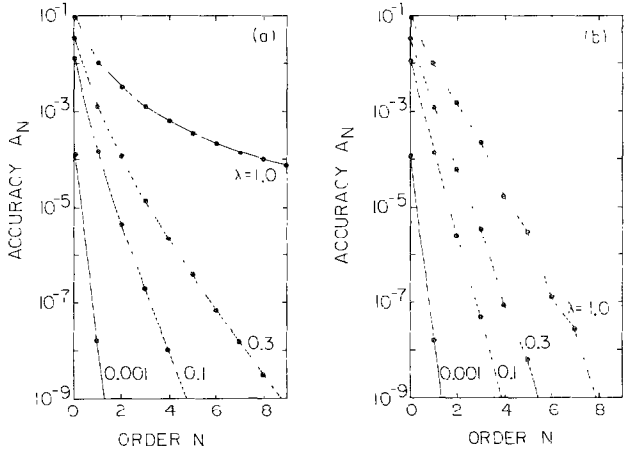

FIG. 2. (a) The accuracy A_N (see Eq. (15)) of series (6) for the anharmonic oscillator with potential $V(x) = \frac{1}{2}x^2 + \lambda x^4$ as a function of the series order N. The four values $\lambda = 0.001$, 0.1, 0.3, and 1.0 are

monic cases ($\lambda \simeq 0$, $\alpha \simeq -\lambda E$) and least effective in the nearly pure anharmonic cases ($\lambda \simeq 1$, $\alpha \simeq -1$). However, even in the pure anharmonic case, (6) is effective in low order, order one is good to 1%, e.g., and the accuracy improves with order. Second, considered overall, the accuracy of (6) is exceptionally good. Even the low orders ($N = 0, 1, 2$) provide fine accuracy. Third, Fig. 2a is for energy $E = 1.0$ only. The restriction to $E = 1.0$ is no loss of generality, however, since the full range of λ values is shown.

As discussed in Section II, the Shanks transformation is a powerful technique for obtaining information from divergent series. The transformation is useful also, however, on series that converge slowly. Thus, we apply the Shanks transformation to the series (6) for the anharmonic oscillator, and we expect the transformation to be most useful for the nearly pure anharmonic cases ($\lambda \simeq 1$, $\alpha \simeq -1$) where the α values are the largest. For order two, expression (12) is used, and for higher orders the transformation is iterated [12]. In Fig. 2b are shown the results of applying the Shanks transformation to series (6) for the same energy and λ values that were used in Fig. 2a; thus Figs. 2a and b can be directly compared. As expected, the transformation does not improve the accuracy of (6) where (6) is already extremely accurate (smaller λ, α), but it does significantly improve the accuracy for the larger λ values. Comparing the $\lambda = 1.0$ curves in Figs. 2a and b indicates that the Shanks transformation produces much higher accuracy especially for the larger orders. For order eight, e.g., the accuracy has been improved from one part in 10^4 to one part in 10^8.

The anharmonic oscillator can be used to illustrate another feature of the basic AVPT equations (1)–(6). From (5) we note that the expansion coefficient $b(1, r)$, which is used in (6), contains x_2 and $u(r)$. Since, in general, both x_2 and $u(r)$ are functions of α, one has that the expansion (6) of $J(E)$ is not a pure expansion in powers of α because the $b(1, r)$ contain α.

We illustrate the physical content of the above observation by considering the anharmonic oscillator with the potential $V(x) = x^2 + \lambda x^4$, which differs slightly from the potential considered earlier. The turning points are given by the previous formulae with the one change $\lambda_1 = 1$. Now, consider zeroth order as given by (8). Since x_2 contains λ (or, equivalently, α), it is clear that zeroth order is not the pure oscillator case $\lambda = 0$. In other words, zeroth order still contains λ. In this sense, AVPT as given by (1)–(6) differs from traditional perturbation theories for which zeroth order means the pure oscillator case $\lambda = 0$. The result is that zeroth order in AVPT is more powerful than zeroth order in traditional theories because a substantial part of the impact of the λx^4 term is already included. This remark holds true for the higher order terms in (6) also, so that in any order the AVPT contains more of the effect of the λx^4 term than the traditional perturbative analyses.

In order to illustrate numerically the effect of the α dependence in the expansion coefficients $b(1, r)$ using the anharmonic oscillator $V(x) = x^2 + \lambda x^4$, we compare the "impure α" expansion (6) of AVPT to a "pure α" expansion which we obtain as follows. At the start of this section it was shown that for the anharmonic oscillator $u(r) = c(r)$, so that by (5), $b(1, r) = \sqrt{E}\, x_2 c(1 + r)\, c(r)$. For the anharmonic

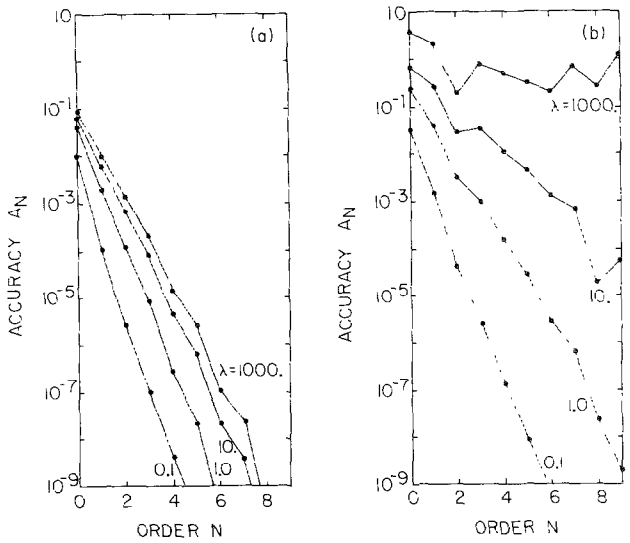

FIG. 3. (a) The accuracy A_N (see (15)) of series (6) for the anharmonic oscillator with potential $V(x)=x^2+\lambda x^4$ as a function of series order N. Four λ values are shown: $\lambda=0.1$, 1.0, 10, and 1000; the Shanks transformation is used on (6) for the latter three λ values. (b) The same as (a) except the "pure α" expansion is used instead of (6) (see Section III).

oscillator with potential $x^2+\lambda x^4$ it can be shown that $x_2=\sqrt{E}\sqrt{1+\alpha}$. Thus, $b(1,r)=E\sqrt{1+\alpha}\,c(1+r)c(r)$, and using this in (6) one has $J_N=-E\sqrt{1+\alpha}\sum c(1+r)\,c(r)\,\alpha^r$, where the sum is over $r=0$ to N. Expanding the factor $\sqrt{1+\alpha}$ in powers of α, inserting this expansion in the expression for J_N, and collecting powers of α, yields $J_N=-\sum \tilde{b}(1,r)\,\alpha^n$, where again the sum is over $r=0$ to N. The expression for $\tilde{b}(1,r)$ is $\tilde{b}(1,r)=E(-1)^r\sum(-1)^k\,c(r-k)\,c(1+k)\,c(k)$, where the sum is over $k=0$ to r. Since the $\tilde{b}(1,r)$ do not contain α, we refer to the $\tilde{b}(1,r)$ expansion of J_N as the "pure α" expansion in contrast to (6), which is called the "impure α" expansion of J_N because the expansion coefficients $b(1,r)$ contain α.

We compare the "impure α" expansion to the "pure α" expansion, which is more like traditional perturbation theories, in Fig. 3. In Fig. 3a are shown the results of (6) for the anharmonic oscillator for $E=1.0$ and $\lambda=0.1$, 1.0, 10.0, and 1000. (These λ values correspond to $-\alpha=0.084$, 0.38, 0.73, and 0.97, respectively.) In Fig. 3b are shown the results of the "pure α" expansion for the same E and λ values. As expected, for small λ (and α) the two series perform similarly. For large λ (and α) however, the AVPT form (6) significantly out-performs the "pure α" expansion; the comparison is particularly striking for $\lambda=1000$, where (6) is effective and the "pure α" expansion fails. The conclusion is that including α dependence in the expansion coefficients $b(1,r)$, as is done in the AVPT expansion (6), results in a perturbation theory which is more effective than the usual pure-expansion-type theories.

IV. Resonance Well

As a second illustration of AVPT we examine the resonance-type potential well $V(x) = -V_0 a^2/(x^2 + a^2)$, where V_0 and a are positive real constants. [This well does not obey the condition $V(0) = 0$ as was assumed in the formulae of Section II; however, the formulae of II remain valid if one replaces $\sqrt{E}$ by $\sqrt{E + V_0}$ in (3), (5), and (8) (and elsewhere as appropriate).] Using the standard form (3) (with E replaced by $E + V_0$) gives $f(x) = (1 + x^2/a^2)^{-1/2}$ with $x_2 = [-(E + V_0) a^2/E]^{1/2}$. Putting $f(x)$ in the standard form (4) and expanding gives $f(x) = (1 - \alpha x^2/x_2^2)^{-1/2} = \sum d(k) \alpha^k (x^2/x_2^2)^k$, where $k = 0, 1, 2, \ldots$, $d(k)$ is the reciprocal square root expansion coefficient, and the natural choice $\alpha = -x_2^2/a^2$ is made. Comparing this expansion of $f(x)$ with (4) gives $u(k) = d(k)$. The definitions of x_2, α, and $u(k)$ used in (5), (6) completes the solution of the resonance-well system.

The resonance-well momentum function $p(x, E)$ has four branch points: x_1, x_2, ia, and $-ia$. The branch points and associated cuts are shown in Figs. 1b and c. The branch points at $\pm ia$ are fixed, but the physical turning points x_1 and x_2 move with energy. For E near the bottom of the well ($E \simeq -V_0$), x_1 and x_2 are small relative to a (Fig. 1b). For E near the top of the well ($E \simeq 0$), x_1 and x_2 are large relative to a (Fig. 1c). In all cases the contour C used in (1) to define $J(E)$ encloses the cut from x_1 to x_2.

In the case of the anharmonic oscillator discussed in Section III, the expansion parameter α was restricted in magnitude to the range $0 \leqslant -\alpha \leqslant 1$. In the case of the resonance well, however, the magnitude of α is not restricted. From the definitions of x_2 and α one has $\alpha = -x_2^2/a^2 = (E + V_0)/E$. Thus, $-\alpha$ increases from 0 to 1 to ∞ as E increases from $-V_0$ to $-V_0/2$ to 0.

The size of α is correlated with the region of validity of expansion (5) for $p(x, E)$. For the resonance well the nearest singularity of $p(x, E)$ outside of x_2 is at ia (see Figs. 1b and c). Thus, expansion (5) is valid in a ring with inner radius x_2 and outer radius a. But $-\alpha = x_2^2/a$, so when $0 \leqslant -\alpha < 1$, (5) has a finite region of validity, whereas when $1 < -\alpha < \infty$, (5) has no region of validity. In the latter range of α values one can ask if (5) and (6) are of any use at all. As will be seen below (5) and (6) remain useful even for large α.

In Fig. 4a are shown the results of series (6) for $J_N(E)$ for the resonance well with parameters $V_0 = 1.$, $a = 1$. Four α values are shown: $-\alpha = 0.02$, 1.0, 10., 50., which correspond to energies $-E = 0.980$, 0.500, 0.0909, 0.0196, respectively. (The Shanks transformation is used on (6) when $N \geqslant 2$ for the latter three α values.) For $\alpha = -0.02$ (6) is highly effective even in zeroth order. For $\alpha = -1.0$ (6) is again effective. For $\alpha = -10$ and -50, which are very large α values corresponding to energies near the top of the well, (6) remains effective if one goes to higher order. To achieve one percent accuracy, e.g., one needs $N = 6$ and 10 for $\alpha = -10$ and -50, respectively. In low order, (6) is not useful for extremely large α values. Thus, (5) and (6) remain useful even when expansion (5) no longer has a region of validity in the x plane. In summary, the AVPT series (6) is effective in an analysis of the resonance well over the full range of energy.

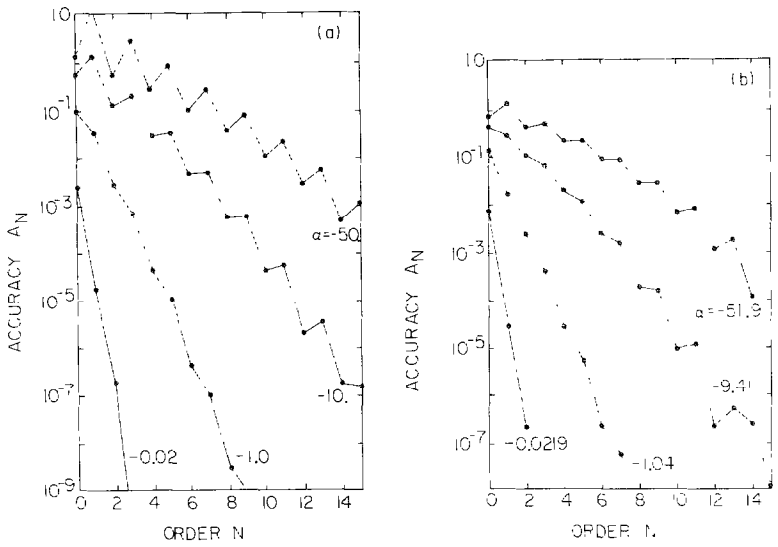

FIG. 4. (a) The accuracy A_N (see (15)) of series (6) for the resonance well $V(x) = -V_0/(x^2 + a^2)$ with $V_0 = a = 1.0$ as a function of series order N. Four values of the expansion parameter α are shown: $\alpha = -0.02$, -1.0, -10, and -50. These α values correspond to various energies (see Section IV). (b) The accuracy of series (17) for the radial effective potential $-g/r + \lambda r + L^2/r^2$ with $g = 2.0$, $\lambda = 0.01$, and $L = 1.0$ as a function of series order N. Four values of α are shown: $\alpha = -0.0219$, -1.04, -9.41, and -51.9, which correspond to various energies (see Section V).

The anharmonic oscillator and resonance potential wells considered in Section II and in this section are simple algebraic functions. However, the AVPT equations of Section II apply equally well to other potentials such as $V(x) = -V_0 \exp(-x^2/a^2)$. For this potential one puts $p(x, E)$ in the standard form and expands $f(x)$ as usual to find $u(k)$. x_2 is given by $x_2^2 = -a^2 \ln(-E/V_0)$ and a natural choice for α is $\alpha = -x_2^2/a^2$. Other potentials are handled similarly.

V. SPHERICALLY SYMMETRIC SYSTEMS

For a particle moving in three dimensions under a spherically symmetric potential $V(r)$, the Hamilton-Jacobi equation separates in spherical polar coordinates r, θ, ϕ [4–6]. The radial action variable J_r, which gives the frequency of the bound-state radial motion, is given by definition (1) with $p(x, E)$ replaced by the radial momentum function $p(r, E, L) = [E - V(r) - L^2/r^2]^{1/2}$. L, the angular momentum, is the sum of the θ and ϕ action variables: $L = J_\theta + J_\phi$. The contour C in (1) encloses the two physical turning points r_1 and r_2 and the cut running between them; see, e.g., Figs. 1d and e. When C is distorted, it picks up a contribution $-L$ from the pole of $p(r, E, L)$ at the origin. Thus, $J_r = -L + J_\infty$, where J_∞ is the con-

tribution to J_r from the other singularities of $p(r, E, L)$. From here on, one proceeds along lines similar to the one-dimensional analysis of Section II.

As our third numerical illustration of the use of AVPT, the potential $V(r) = -g/r + \lambda r$ is analyzed. (λ and g are positive, real constants.) The momentum function is $p(r, E, L) = [E + g/r - \lambda r - L^2/r^2]^{1/2}$, and the system has three turning points r_1, r_2, and r_3 such that $0 < r_1 < r_2$ and $r_3 < 0$. (r_3 is unphysical; for small λ, $r_3 \simeq E/\lambda$.) $p(r, E, L)$ can be written in the form $p(r, E, L) = i\sqrt{-\lambda r_3}(1 - r_1/r)^{1/2}(1 - r_2/r)^{1/2}(1 - r/r_3)^{1/2}$. Expanding the three square roots yields

$$p(r, E, L) = i \sum_{s=0}^{\infty} \sum_{n=-s}^{\infty} b(n, s)\, \alpha^s r^{-n},$$
$$b(n, s) = \sqrt{-\lambda r_3}\, r_2^n c(s) \sum_{k=0}^{n+s} c(k)\, c(n+s-k)(r_1/r_2)^k, \tag{16}$$

with $\alpha = r_2/r_3$. Expansion (16) is valid in the region $r_2 < |r| < -r_3$. Using (16) in (1), and remembering that J_r has the contribution $-L$ from the pole of $p(r, E, L)$ at the origin, gives

$$J_{rN}(E, L) = -L - \sum_{s=0}^{N} b(1, s)\, \alpha^s \tag{17}$$

which completes the AVPT solution of this system. (17) is the radial analog of series (6) for the one-dimensional $J_N(E)$. (Note that to use (17) it is necessary to obtain the turning points r_1, r_2, and r_3.)

Since (16) and (17) are valid in the r-plane region $r_2 < |r| < -r_3$, we see that (16) and (17) are valid when $r_2 < -r_3$ and $0 < -\alpha < 1$ (see Fig. 1d), and invalid when $r_2 > -r_3$ and $1 < -\alpha < \infty$ (see Fig. 1e). However, as in the case of the resonance well, (16) and (17) provide useful information even for $1 < -\alpha < \infty$ as we see below.

In Fig. 4b are shown the results of applying AVPT series (17) to the radial effective potential $V(r) + L^2/r^2 = -g/r + \lambda r + L^2/r^2$. The figure is for $g = 2.0$, $\lambda = 0.01$, $L = 1.0$, and various E values. For these g, λ, and L values the bottom of the effective potential well is at -0.999 and the E values shown run from just above the bottom of the well to large, positive E. Four values of α are shown: $\alpha = -0.0219$, -1.04, -9.41, and -51.9, which correspond to the energies $E = -0.790$, 0.00998, 0.410, 1.11, respectively. (The Shanks transformation is used for the latter three α values for order $N \geqslant 2$.) As usual, the theory is highly effective for small α values such as $\alpha = -0.0219$. For $\alpha = -1.04$, which is not small, the series (17) is still highly effective even in low order. For the large α values, -9.41 and -51.9, it is seen in Fig. 4b that good accuracy is possible, but only in higher order. To achieve 1% accuracy, e.g., one must go to $N = 5$ and 10 for $\alpha = -9.4$ and -51.9, respectively. Series (17) is not useful in low order for the very large α values. These results parallel those found earlier for the resonance well.

In Fig. 4b it is seen that AVPT series (17) provides a good basis for analyzing the three-dimensional system with radial effective potential $-g/r+\lambda r+L^2/r^2$ and $g=2.0$, $\lambda=0.01$, and $L=1.0$. However, (17) is effective also for other values of the potential parameters g and λ. Large values of λ such as 2.0 or 4.0 or larger can be handled. In addition, small values of g can be treated, including the case $g=0$. For $g=0$ there are still the three turning points r_1, r_2, and r_3, and Eqs. (16) and (17) remain valid. Lastly, (16) and (17) remain intact for the case $L=0$: in this case $r_1=0$ and the sum in $b(n, s)$ reduces to its first term only. In summary, (17) is effective for a wide range of g, λ, and L values.

The radial motion under potential $V(r)=-g/r+\lambda r$ was analyzed above; however, it is clear that related potentials can be treated similarly. For other potentials, (17) and the $p(r, E, L)$ expansion in (16) remain valid. Different systems have, in general, different expressions for $b(n, s)$ and for α. The specific forms for $b(n, s)$ and α depend upon the location and nature of the singularities of $p(r, E, L)$, which in turn depend upon $V(r)$.

VI. Additional Spherically Symmetric Systems

In the above analysis of the radial potential $V(r)=-g/r+\lambda r$, the term λr can be viewed as perturbing the coulomb term $-g/r$. This perturbation occurs near $r=\infty$, where λr is significant; e.g., we saw above that $r_3\simeq E/\lambda$ for small λ so r_3 is far out on the negative real r axis as shown in Fig. 1d. For other potentials, however, a "perturbing" term may be significant at some other point in the r plane besides $r=\infty$. An example is the potential $V(r)=-g/r+\lambda/r^3$, which can be viewed as a spin-orbit-type interaction λ/r^3 perturbing the coulomb term $-g/r$. λ/r^3 makes itself felt near $r=0$ so that $p(r, E, L)$ is no longer $\simeq -iL/r$ near $r=0$. Thus, the contribution to the J_r integral from the $r=0$ region is no longer $-L$ (see, e.g., (17)), but is instead a more complicated term which reduces to $-L$ as λ goes to zero. In the following we outline the solution for the potential $V(r)=-g/r+\lambda/r^3$; this solution complements the earlier solution of $V(r)=-g/r+\lambda r$ in Section V.

For $V(r)=-g/r+\lambda/r^3$ (g, λ are real and positive) the momentum function is $p(r, E, L)=[E+g/r-\lambda/r^3-L^2/r^2]^{1/2}$. The system has the usual two physical turning points r_1 and r_2 with $0\leqslant r_1<r_2$, and, in addition, a third, unphysical, turning point r_3 on the negative real r axis. For λ small, $r_3\simeq -\lambda/L^2$. Also, $r=0$ is now a branch point of $p(r, E, L)$, since $p(r, E, L)\simeq[-\lambda/r^3]^{1/2}$ near $r=0$. Thus, we let $p(r, E, L)$ have a cut running from r_3 to $r=0$ on the negative real r axis. When the contour C in (1) is distorted it encloses this cut producing a contribution J_0 to the J_r integral. In addition to the J_0 contribution which comes from the $r=0$ region, there is a contribution to J_r from $r=\infty$ where the integrand of (1) has a pole. This latter contribution is easily obtained and is $g/2\sqrt{-E}$. Thus, $J_r(E, L)=J_0(E, L)+g/2\sqrt{-E}$.

Action-variable perturbation theory can be used to calculate J_0 as follows. $p(r, E,$

L) can be put in the form $p(r, E, L) = (Er_1r_2/r^2)^{1/2}(1-r/r_1)^{1/2}\ (1-r/r_2)^{1/2}(1-r_3/r)^{1/2}$. Expanding the last three square roots gives

$$p(r, E, L) = \frac{i}{r}\sum_{s=0}^{\infty}\sum_{n=-s}^{\infty} b(n, s)\,\alpha^s r^{-n},$$
$$b(n, s) = -\sqrt{-Er_1r_2}\, r_3^n c(n+s)\sum_{k=0}^{s} c(k)\,c(s-k)(r_1/r_2)^k, \tag{18}$$

where $\alpha = r_3/r_1$. Equation (18) is valid in the region $-r_3 < |r| < r_1$, i.e., when $-\alpha < 1$. Now, since a piece of the contour C encloses the region near $r=0$ as discussed above, the first-order pole term of expansion (18) produces J_0. Thus, from (18),

$$J_{rN}(E, L) = J_{0N}(E, L) + g/2\sqrt{-E}$$
$$= \sum_{s=0}^{N} b(0, s)\,\alpha^s + g/2\sqrt{-E} \tag{19}$$

to order N. Series (19) for the perturbation near $r=0$ is the analog of series (17) for the perturbation near $r=\infty$. (19) completes the $AVPT$ solution for the three-dimensional system with potential $V(r) = -g/r + \lambda/r^3$. (We do not illustrate (19) numerically because the results parallel the earlier illustration done with (17).)

From the discussion of this and the previous section. it is clear that systems which require expansions both near $r=0$ and $r=\infty$ are easily treated. Obvious examples are $V(r) = -g/r + \lambda_1/r^3 + \lambda_2 r$ and $V(r) = \lambda_1/r^3 + \lambda_2 r$. The essential point is that $p(r, E, L)$ is expanded near $r=0$ and $r=\infty$, and appropriate terms in the expansions are used to evaluate the integral (1).

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