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New theorem on action integrals and oscillation periods of motion in polynomial multi-well potentials

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Abstract. The present theoretical investigation shows that the oscillation periods and the corresponding classical action integrals, associated with motion of a given energy in the local wells of a multi-well anharmonic potential, are linearly dependent. The proof makes use of the analytic behaviour of the local momentum of the particle in the complex position variable. The theorem applies to polynomial potentials of arbitrary even degree.

1. Introduction

Anharmonic potential models have a wide range of applications in physics and chemistry (Nayfeh and Mook 1979, Hayashi 1985), and have been studied in detail by many scientists. In a recent numerical work, Ali and Snider (1989) discovered some less familiar properties of classical quartic, sextic and octic oscillators. The main purpose of the present paper is to show, quite generally, the conjectures put forward (and numerically verified in three cases) by Ali and Snider. Consider a one-dimensional motion of a point mass in a polynomial potential of even degree $n = 4, 6, 8, \ldots$, with the potential parameters and the total mechanical energy given such that all classical turning points are real valued, i.e. there are $n/2$ separated wells in which the classical motion is possible. For a system satisfying these conditions the oscillation periods $(T_1, T_2, \ldots)$ pertaining to the local wells are linearly dependent, satisfying the relation

$$T_1 - T_2 + T_3 - \ldots - (-1)^{n/2} T_{n/2} = 0. \tag{1}$$

For an arbitrary quartic potential ($n = 4$) this result implies that the period in one well is equal to that in the other well. Since the potential wells are generally asymmetric it is not directly realized why the periods should be equal. Note, however, that the local periods T_j are in general energy dependent, in contrast to the harmonic oscillator case $n = 2$.

Ali and Snider (1989) give an explicit formula for the periods T_1 and T_2 for the case $n = 4$, and the authors indicate the existence of an analytic proof of the relation (1) also for the cases $n = 6$ and 8, involving hyperelliptic integrals.

In the present paper I shall outline a proof of equation (1) for the general case, using complex analysis. In section 2 I define the anharmonic oscillator model. Section 3 deals with the proof of equation (1) and conclusions are given in section 4.

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2. The anharmonic oscillator model

I consider the motion of a particle given by the one-dimensional Hamiltonian

$$H = p^2/2 + V(x) \tag{2}$$

where p is the linear momentum, and $V(x)$ is the potential of a given analytic form

$$V(x) = \sum_{j=1}^{n} D_j x^j \qquad n = 4, 6, 8, \ldots. \tag{3}$$

The potential in equation (3) is slightly more general than that discussed by Ali and Snider (1989) in the sense that the linear term is included in the present treatment.

The mechanical energy E is identical to the Hamiltonian H in the present model. For the time being I shall assume that the potential parameters D_j are such that all classical turning points are real and that the coefficient pertaining to the highest power of the potential, i.e. D_n, is positive. In section 4 I discuss the more general case when classical turning points are complex valued.

With a slightly different notation to that used by Ali and Snider, we write the period of oscillation of a particle in the jth local well (counting from the left along the real x axis) as

$$T_j = \sqrt{2} \int_{a_j}^{b_j} \frac{\mathrm{d}x}{(E - V(x))^{1/2}} \tag{4}$$

where E is the conserved mechanical energy. In the following section I shall make use of the well known relation between the period and the action integral:

$$T_j = 2\pi \, \mathrm{d}I_j/\mathrm{d}E \tag{5}$$

where

$$I_j = (\sqrt{2}/\pi) \int_{a_j}^{b_j} (E - V(x))^{1/2} \, \mathrm{d}x. \tag{6}$$

3. Derivations

The proof of equation (1) follows a semiclassical technique used in quantum mechanics by Sommerfeld (1969) and it is organized in the following way. Firstly, I define a generalized action integral $\Im_n$, the *global action*, which is defined along a closed contour in the complex x plane circumventing all classical turning points. Secondly, I show the following linear relation for the local action integrals:

$$\sum_{j=1}^{n/2} (-1)^{j+1} I_j = \Im_n. \tag{7}$$

Thirdly, I proceed to construct a recursion scheme for the determination of explicit algebraic expressions for the global action $\Im_n$ on the right-hand side of equation (7). Finally, from the property of these recursion relations, I conclude that $\Im_n$ is an energy-independent quantity when $n > 2$. Clearly equation (1) then follows from (7) and (3).

3.1. *Definition of the global action integral*

The analytic definition of the global action is based on the proper analytic behaviour of the local momentum $\sqrt{2}(E - V(x))^{1/2}$ in the complex coordinate plane. The local momentum is made single valued by introducing cuts emerging from the turning points, which are branch point singularities. For simplicity, I deform the cuts in such a way that they cancel everywhere in the complex plane, except on the real axis in the classically allowed regions of the potential.

I then define the global action as the contour integral

$$\Im_n = \frac{1}{2}\int_C \frac{\sqrt{2}}{\pi}(E - V(x))^{1/2}\,\mathrm{d}x \tag{8}$$

where C is a closed contour circumventing all the turning points in the negative sense (see figure 1). As can be seen in figure 1, the contour C does not cross any cuts.

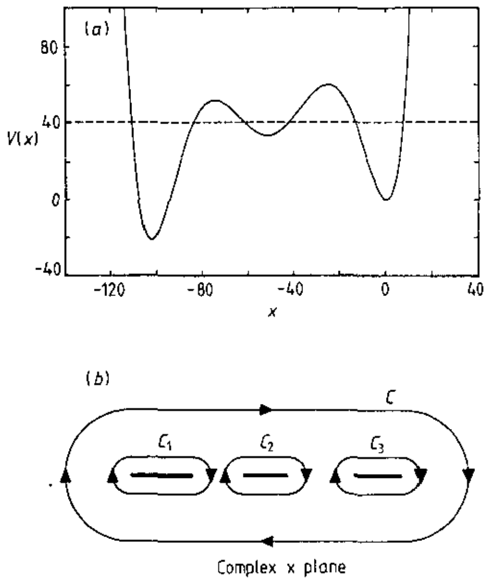

Figure 1. *The figure shows (a) the potential energy diagram for the sextic anharmonic oscillator* (see Ali and Snider (1989) for details) and (*b*) the pertinent complex contours defining the action integrals.

3.2. *Derivation of equation (7)*

It is now a simple matter to split the contour C into a set of closed contours C_j circumventing each cut (local well). Equation (7) then follows from the fact that the local momentum is positive on the upper lip of the odd-labelled cuts, and negative on the upper lip of the even-labelled cuts.

3.3. *Evaluation of the global action integral*

To show that $\Im_n$ is energy independent I proceed to evaluate the defining contour integral by residue calculus.

Let C lie sufficiently far away from the turning points and the origin. To construct a MacLaurin expansion of the integrand in (8), I factorize out the leading term in the argument of the square root, thus obtaining

$$(E - V(x))^{1/2} = \mathrm{i}\sqrt{D_n}(-1)^{n/2}x^{n/2}\left(\frac{V(x) - E}{D_n x^n}\right)^{1/2} \tag{9}$$

so that the phase factor of the integrand in (8) becomes i for large negative values of x, i.e. for $x = -|x|$. Note that D_n is assumed positive. To complete the expansion I write

$$\frac{V(x) - E}{D_n x^n} = 1 + \sum_{j=1}^{n} a_j x^{-j} \tag{10}$$

with

$$\begin{aligned} a_m &= D_{n-m}/D_n \qquad \text{for } m = 1, 2, \ldots, n-1 \\ a_n &= E/D_n. \end{aligned} \tag{11}$$

I define a new set of expansion coefficients b_m through the relation

$$\left(1 + \sum_{j=1}^{n} a_j x^{-j}\right)^{1/2} = \sum_{m=0}^{\infty} b_m x^{-m} \tag{12}$$

which, by repeated expansions of multinomials, leads to the following formula:

$$b_m = \sum_{j=0}^{m} \binom{1/2}{j} a_m^{(j)} \tag{13}$$

where the coefficients $a_m^{(j)}$ are determined by the recursion relation

$$a_m^{(j+1)} = \sum_{k=j}^{m-1} a_k^{(j)} a_{m-k} \tag{14}$$

with

$$\begin{aligned} a_m^{(0)} &= \begin{cases} 1 & m = 0 \\ 0 & m > 0 \end{cases} \\ a_m^{(1)} &= a_m \qquad m \geqslant 1. \end{aligned} \tag{15}$$

The action integral $\Im_n$ can now be evaluated by the residue theorem. I find

$$\Im_n = \sqrt{2D_n}(-1)^{n/2} b_{n/2+1} \tag{16}$$

where n is an even integer. For $n = 2$, 4, 6 and 8, the relevant coefficients b_2, b_3, b_4 and b_5, respectively, are given by

$$b_2 = \tfrac{1}{2}a_2 - \tfrac{1}{8}a_1^2 \tag{17}$$

$$b_3 = \tfrac{1}{2}a_3 - \tfrac{1}{8}(2a_1a_2) + \tfrac{1}{16}a_1^3 \tag{18}$$

$$b_4 = \tfrac{1}{2}a_4 - \tfrac{1}{8}(2a_1a_3 + a_2^2) + \tfrac{1}{16}(3a_1^2a_2) - \tfrac{5}{128}a_1^4 \tag{19}$$

$$b_5 = \tfrac{1}{2}a_5 - \tfrac{1}{8}(2a_1a_4 + 2a_2a_3) + \tfrac{1}{16}(3a_1^2a_3 + 3a_2^2a_1) - \tfrac{5}{128}(4a_1^3a_2) + \tfrac{35}{1280}a_1^5 \tag{20}$$

where the a_m are defined in equation (11).

In terms of the original parameters of the Hamiltonian I find

$$\Im_2=-\left(\frac{D_2}{2}\right)^{1/2}[E/D_2-\tfrac{1}{4}(D_1/D_2)^2] \tag{21}$$

$$\Im_4=\left(\frac{D_4}{2}\right)^{1/2}[D_1/D_4-\tfrac{1}{4}(2D_3D_2)/D_4^2+\tfrac{1}{8}(D_3/D_4)^3] \tag{22}$$

$$\Im_6=-\left(\frac{D_6}{2}\right)^{1/2}[D_2/D_6-\tfrac{1}{4}(2D_5D_3+D_4^2)/D_6^2+\tfrac{1}{8}(3D_5^2D_4)/D_6^3-\tfrac{5}{128}(D_5/D_6)^4] \tag{23}$$

$$\Im_8=\left(\frac{D_8}{2}\right)^{1/2}[D_3/D_8-\tfrac{1}{4}(2D_7D_4+2D_6D_5)/D_6^2+\tfrac{1}{8}(3D_7^2D_5+3D_7D_6^2)/D_6^3$$
$$-\tfrac{5}{128}(4D_7^3D_6)/D_8^4+\tfrac{35}{1280}D_7^5]. \tag{24}$$

As is clearly seen in the expressions (21)–(24) above, the global action is energy dependent only for the harmonic oscillator potential (with $n=2$). The general proof of the energy independence of the global action integral for $n>2$ follows by examining equations (11), (13)–(16). In short, the expression for $\Im_n$ will only contain expansion coefficients a_m, with $m=1,2,\ldots,n/2+1$, whilst the energy appears in a_n.

4. Discussion

To prove equation (1) by explicit evaluation of the local oscillation periods is difficult, involving a great deal of working experience with hyperelliptic integrals. However, once it has been defined, the global action integral is far more easy to evaluate and the proof of (1) follows from (7). The physical significance of the global action integral, as defined in the present paper, is appreciated in the field of phase-integral methods (Sommerfeld 1969, Berry and Mount 1972) for solving the Schrödinger equation in quantum mechanics.

I have performed a numerical test of the expression for $\Im_6$ and $\Im_8$ in equations (23) and (24), respectively, for the particular sextic and octic potentials given in Ali and Snider (1989). From their tables of numerically computed local action integrals I find, using relation (7), the value 95.148 364 86 for $\Im_6$ and −131.085 7368 for $\Im_8$. A direct use of formulae (23) and (24) give the numerical results 95.148 364 8601 and −131.085 736 828, respectively.

Mathematically, the relations (1) and (7) still hold if the classical turning points become complex valued. However, the classical meaning of the present results in such a situation is unclear. For example, with an increase of the total energy, a particle moving in one of two wells of a quartic potential may suddenly be able to oscillate back and forth in a double well with a certain period T. The local periods T_1 and T_2 are now complex valued, still satisfying $T_1=T_2$ according to equation (1), but they have no obvious meaning in classical mechanics even if one can show that $T=\mathrm{Re}(T_1+T_2)$ is mathematically valid.

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