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Reversion of generalized hypergeometric functions and the application to anharmonic oscillators

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Abstract. Initially, the canonical form $H(J)$ of the Hamiltonian $H(q,p)=\frac{1}{2}p^2+\frac{1}{2}\omega_0^2q^2+\lambda q^\alpha$ ($\omega_0, \lambda \in \mathbb{R}$ and $\alpha > 2$), which represents a large class of anharmonic oscillators, is expressed in a closed form. This is a new result, as is the subsequent closed form of the pulsation $\omega(J)$. The connection between series reversion and inversion, as applied to generalized hypergeometric functions, is also considered and extended to apply to arbitrary series.

1. Introduction

The technique of series reversion has been used to obtain the canonical form $H(J)$ of the Hamiltonian $H(q,p)=\frac{1}{2}p^2+\frac{1}{2}\omega_0^2q^2+\lambda q^\alpha$ ($\omega_0, \lambda \in \mathbb{R}$ and $\alpha > 2$) for many years. It has not previously been possible, however, to obtain a closed expression for this due to the complexity of generalized hypergeometric functions. This problem has been addressed before (Cadaccioni and Caboz 1984) but without success. In this paper, we use the Lagrange expansion (Abramowitz and Stegun 1965, equation (3.6.6)) and combinatorial analysis in an original manner to obtain the elusive closed form of $H(J)$ and also the pulsation $\omega(J)$.

The connection between series reversion and inversion, also noted by Cadaccioni and Caboz (1984), is considered by viewing the Lagrange expansion in a slightly different way. In the concluding section, this connection is considered for a general function $y(x)$ and the convergence properties of $H(J)$ and $\omega(J)$ are also investigated.

2. The canonical form of the Hamiltonian

It is known that the period and the action variable can be expressed in the following way (Codaccioni and Caboz 1984, 1985):

$$T(h)=\frac{2\pi}{\omega_0}\,{}_{\frac{\alpha}{2}}F_{\frac{\alpha}{2}-1}\left[\frac{1}{\alpha},\frac{3}{\alpha},\ldots,\frac{\alpha-1}{\alpha};\frac{2}{\alpha-2},\frac{4}{\alpha-2},\ldots,\frac{\alpha-2}{\alpha-2};z\right] \tag{2.1}$$

$$J(h)=\frac{h}{\omega_0}\,{}_{\frac{\alpha}{2}}F_{\frac{\alpha}{2}-1}\left[\frac{1}{\alpha},\frac{3}{\alpha},\ldots,\frac{\alpha-1}{\alpha};\frac{4}{\alpha-2},\frac{6}{\alpha-2},\ldots,\frac{\alpha-2}{\alpha-2},\frac{\alpha}{\alpha-2};z\right] \tag{2.2}$$

for α even and

$$T(h)=\frac{2\pi}{\omega_0}\,{}_{\alpha}F_{\alpha-1}\left[\frac{1}{2\alpha},\frac{3}{2\alpha},\ldots,\frac{2\alpha-1}{2\alpha};\frac{1}{\alpha-2},\frac{2}{\alpha-2},\ldots,\frac{\alpha-2}{\alpha-2},\frac{1}{2};z^2\right] \tag{2.3}$$

$$J(h)=\frac{h}{\omega_0}\,{}_{\alpha}F_{\alpha-1}\left[\frac{1}{2\alpha},\frac{3}{2\alpha},\ldots,\frac{2\alpha-1}{2\alpha};\frac{2}{\alpha-2},\frac{3}{\alpha-2},\ldots,\frac{\alpha-1}{\alpha-2},\frac{1}{2};z^2\right] \tag{2.4}$$

for α odd where

$$z=\frac{-\lambda h^{(\alpha-2)/2}\alpha^{\alpha/2}}{\{(\alpha-2)/2\}^{(\alpha-2)/2}\omega_0^{\alpha}}. \tag{2.5}$$

These expressions were initially determined heuristically (Caboz and Poletti 1983, Caboz and Loiseau 1983, Caboz 1983). Since then, they have been mathematically proven (Loiseau *et al* 1988, 1989) using results obtained by Caboz *et al* (1985). Note that they are only convergent for $|z|<1$ but may be analytically continued for $|z|>1$ for an infinite potential well ($\lambda>0, \alpha$ even).

Therefore, in general,

$$J(h)=\frac{h}{\omega_0}F(h) \tag{2.6}$$

where h is the energy. Using the Lagrange expansion, and remembering that $H(q,p)=h$, we obtain the expression

$$H(J)=\sum_{k=1}^{\infty}\frac{J^k}{k!}\left[\left(\frac{\mathrm{d}}{\mathrm{d}h'}\right)^{k-1}\left\{\frac{h'}{J(h')}\right\}^k\right]_{h'=0} \tag{2.7}$$

$$=\sum_{\kappa=0}^{\infty}\frac{(\omega_0 J)^{\kappa+1}}{(\kappa+1)!}\left[\left(\frac{\mathrm{d}}{\mathrm{d}h'}\right)^{\kappa}\{F(h')\}^{-(\kappa+1)}\right]_{h'=0}. \tag{2.8}$$

It should be explained that this expression is only valid when

$$\left[\frac{\mathrm{d}}{\mathrm{d}h'}(J(h'))\right]_{h'=0}\neq 0 \tag{2.9}$$

but it is clear from equation (2.6) that

$$\left[\frac{\mathrm{d}}{\mathrm{d}h'}(J(h'))\right]_{h'=0}=\frac{1}{\omega_0}\neq 0. \tag{2.10}$$

Now note that

$$\left[\left(\frac{\mathrm{d}}{\mathrm{d}h'}\right)^{\kappa}\{F(h')\}^{-(\kappa+1)}\right]_{h'=0}=\kappa! a_\kappa \tag{2.11}$$

where a_κ is the coefficient of $(h')^\kappa$ in $\{F(h')\}^{-(\kappa+1)}$. By considering $F=F(h')$, we can see that

$$F^{-(\kappa+1)}=[1-(1-F)]^{-(\kappa+1)}={}_1F_0(\kappa+1;\ ;1-F) \tag{2.12}$$

$$=\sum_{m=0}^{\infty}(-1)^m\frac{(\kappa+1)_m}{m!}(F^*)^m \tag{2.13}$$

with F^* defined to be

$$F^*=\sum_{r=1}^{\infty}\left[\left(\frac{1}{\alpha}\right)_r\left(\frac{3}{\alpha}\right)_r\cdots\left(\frac{\alpha-1}{\alpha}\right)_r\right]\Big/\left[\left(\frac{4}{\alpha-2}\right)_r\left(\frac{6}{\alpha-2}\right)_r\cdots\right.$$
$$\left.\cdots\left(\frac{\alpha-2}{\alpha-2}\right)_r\left(\frac{\alpha}{\alpha-2}\right)_r\right]\frac{z^r}{r!}\qquad \alpha\text{ even}$$
$$=\sum_{r=1}^{\infty}\left[\left(\frac{1}{2\alpha}\right)_r\left(\frac{3}{2\alpha}\right)_r\cdots\left(\frac{2\alpha-1}{2\alpha}\right)_r\right]\Big/\left[\left(\frac{2}{\alpha-2}\right)_r\left(\frac{3}{\alpha-2}\right)_r\cdots\right.$$
$$\left.\cdots\left(\frac{\alpha-1}{\alpha-2}\right)_r\left(\frac{1}{2}\right)_r\right]\frac{z^{2r}}{r!}\qquad \alpha\text{ odd}. \tag{2.14}$$

Now $F^{-(\kappa+1)}$ may be written in the form

$$F^{-(\kappa+1)} = \sum_{m=0}^{\infty}(-1)^m \frac{(\kappa+1)_m}{m!}\left(\sum_{k=1}^{\infty}\frac{x_k}{k!}y^k\right)^m \tag{2.15}$$

$$= \sum_{m=0}^{\infty}(-1)^m(\kappa+1)_m \sum_{r=m}^{\infty}\frac{y^r}{r!}\sum(r;a_1,a_2,\ldots,a_r)'\prod_{j=1}^{r}x_j^{a_j}. \tag{2.16}$$

To obtain this latter expression we note that $\left(\sum_{k=1}^{\infty}(x_k/k!)y^k\right)$ is a generating function for a multinomial expansion of the form given above (see Abramowitz and Stegun 1965, section 24.1.2) where

$$(r;a_1,a_2,\ldots,a_r)' = r!/(1!)^{a_1}a_1!(2!)^{a_2}a_2!\ldots(r!)^{a_r}a_r! \tag{2.17}$$

and is summed over

$$a_1 + 2a_2 + \cdots + ra_r = r \tag{2.18}$$

and

$$a_1 + a_2 + \cdots + a_r = m. \tag{2.19}$$

The other terms in equations (2.16) and (2.17) are defined to be

$$y = \begin{cases} z & \alpha \text{ even} \\ z^2 & \alpha \text{ odd} \end{cases} \tag{2.20}$$

$$x_j = \begin{cases} \left[\left(\frac{1}{\alpha}\right)_j\left(\frac{3}{\alpha}\right)_j\cdots\left(\frac{\alpha-1}{\alpha}\right)_j\right]\Big/\left[\left(\frac{4}{\alpha-2}\right)_j\left(\frac{6}{\alpha-2}\right)_j\cdots\right. \\ \qquad\left.\cdots\left(\frac{\alpha-2}{\alpha-2}\right)_j\left(\frac{\alpha}{\alpha-2}\right)_j\right] & \alpha \text{ even} \\ \left[\left(\frac{1}{2\alpha}\right)_j\left(\frac{3}{2\alpha}\right)_j\cdots\left(\frac{2\alpha-1}{2\alpha}\right)_j\right]\Big/\left[\left(\frac{2}{\alpha-2}\right)_j\left(\frac{3}{\alpha-2}\right)_j\cdots\right. \\ \qquad\left.\cdots\left(\frac{\alpha-1}{\alpha-2}\right)_j\left(\frac{1}{2}\right)_j\right] & \alpha \text{ odd.} \end{cases} \tag{2.21}$$

It can be seen that equation (2.11) holds for

$$\kappa = \begin{cases} \frac{(\alpha-2)}{2}l & \alpha \text{ even} \\ (\alpha-2)l & \alpha \text{ odd} \end{cases} \tag{2.22}$$

where $l = 0, 1, 2, \ldots$ and hence

$$H(J) = \omega_0 \sum_{l=0}^{\infty}\frac{(\eta)^l}{l!}\frac{J^{\kappa+1}}{(\kappa+1)}\sum_{m=0}^{l}(-1)^m(\kappa+1)_m\sum(l;a_1,a_2,\ldots,a_l)'\prod_{j=1}^{l}x_j^{a_j} \tag{2.23}$$

with

$$\eta = \begin{cases} \dfrac{-\lambda\alpha^{\alpha/2}}{\left\{\frac{(\alpha-2)}{2}\right\}^{(\alpha-2)/2}\omega_0^{(\alpha+2)/2}} & \alpha \text{ even} \\ \dfrac{\lambda^2\alpha^{\alpha}}{\left\{\frac{(\alpha-2)}{2}\right\}^{\alpha-2}\omega_0^{\alpha+2}} & \alpha \text{ odd.} \end{cases} \tag{2.24}$$

Similarly, the pulsation may be written in the following closed form:

$$\omega(J) = \frac{\mathrm{d}H}{\mathrm{d}J} = \omega_0 \sum_{l=0}^{\infty} \frac{(\eta)^l}{l!} J^{\kappa} \sum_{m=0}^{l} (-1)^m (\kappa+1)_m \sum (l; a_1, a_2, \ldots, a_l)' \prod_{j=1}^{l} x_j^{a_j}. \tag{2.25}$$

The first eleven non-zero coefficients of J^n in either expression can be obtained by using Abramowitz and Stegun (1965, table 24.2). Shown below (in table 1) are the first eleven terms of ω/ω_0 for the Duffing oscillator ($\alpha = 4, \lambda > 0$).

Table 1. Coefficients of $(\lambda J/(\omega_0^3))^n$ in ω/ω_0 for the Duffing oscillator expressed in terms of a rational number of the form $p/2^q$.

n	p	q
0	1	0
1	3	0
2	−51	2
3	375	2
4	−53 445	6
5	262 647	5
6	−21 926 793	8
7	238 225 977	8
8	−170 513 657 325	14
9	974 520 584 235	13
10	−90 642 576 672 219	16

3. The connection between series reversion and inversion

By retaining the first few terms of the above series, it is possible to show that $2\pi/\omega(h)$ does, in fact, yield the first few terms of the period $T(h)$. In this section, however, we show explicitly that they are entirely equivalent. If we define, for simplicity,

$$G(h) = \frac{\omega_0 T(h)}{2\pi} \tag{3.1}$$

so that

$$\int_0^h G(h')\,\mathrm{d}h' = hF(h) \tag{3.2}$$

where $T(h)$ is given by equations (2.1), (2.3), and $F(h)$ by equation (2.6), then it is possible to write

$$\frac{\omega T}{2\pi} = \frac{\omega}{\omega_0} G(h) \tag{3.3}$$

$$= \sum_{\kappa=0}^{\infty} \frac{(\omega_0 J)^\kappa}{\kappa!} \left[\left(\frac{\mathrm{d}}{\mathrm{d}h'} \right)^\kappa \{F(h')\}^{-(\kappa+1)} \right]_{h'=0} G(h) \tag{3.4}$$

$$= \frac{1}{2\pi \mathrm{i}} \oint^{(0+)} \sum_{\kappa=0}^{\infty} (\omega_0 J)^\kappa \frac{G(h)\,\mathrm{d}h'}{[h'F(h')]^{\kappa+1}} \tag{3.5}$$

$$= \frac{1}{2\pi \mathrm{i}} \oint^{(0+)} \sum_{\kappa=0}^{\infty} \frac{[hF(h)]^\kappa}{[h'F(h')]^{\kappa+1}} \frac{\mathrm{d}}{\mathrm{d}h} [hF(h)]\,\mathrm{d}h' \tag{3.6}$$

$$= \frac{1}{2\pi \mathrm{i}} \frac{\mathrm{d}}{\mathrm{d}h} \oint^{(0+)} \sum_{\kappa=0}^{\infty} \frac{1}{(\kappa+1)} \left[\frac{hF(h)}{h'F(h')} \right]^{\kappa+1} \mathrm{d}h' \tag{3.7}$$

$$= \frac{-1}{2\pi \mathrm{i}} \frac{\mathrm{d}}{\mathrm{d}h} \oint^{(0+)}_{|h'|>|h|} \ln \left[1 - \frac{hF(h)}{h'F(h')} \right] \mathrm{d}h'. \tag{3.8}$$

The last step is reliant on the inequality $|h'F(h')| > |hF(h)|$ being satisfied. This can be achieved by choosing $|h'|$ sufficiently large which then involves analytic continuation of $F(h')$. Hence it is necessary to generalize the Abramowitz and Stegun (1965) equation (15.3.7) for a general ${}_pF_q$ where $p = q + 1$. This is given by

$$\begin{aligned} {}_pF_q \left[\begin{matrix} a_1, a_2, a_3, \ldots, a_p; \\ b_1, b_2, \ldots, b_q; \end{matrix} \quad z \right] &= \sum_{n=1}^{p} (-z)^{-a_n} \prod_{\substack{m=1 \\ m \neq n}}^{p} \frac{\Gamma(a_m - a_n)}{\Gamma(a_n)} \prod_{l=1}^{q} \frac{\Gamma(b_l)}{\Gamma(b_l - a_n)} \\ &\quad \times {}_pF_q \left[\begin{matrix} a_n, c_1, c_2, \ldots, c_q; \\ d_1, d_2, \ldots, d_{n-1}, d_{n+1}, \ldots, d_p; \end{matrix} \quad z^{-1} \right] \end{aligned} \tag{3.9}$$

where c_r and d_r are defined to be

$$\begin{aligned} c_r &= 1 + a_n - b_r \\ d_r &= 1 + a_n - a_r \end{aligned} \tag{3.10}$$

and was arrived at by following Copson's (1935) derivation of the analytic continuation for the Gauss hypergeometric function.

If we consider the first term in the summation for the specific ${}_pF_q$ in question, then we find that

$$(z)^{-a_1} \propto (h')^{-(\alpha-2)/(2\alpha)} \qquad \forall \alpha \tag{3.11}$$

and therefore the first term of $h'F(h')$ is proportional to $(h')^{\alpha+2/(2\alpha)}$ for large h'. Thus, it is apparent that the contour of integration can always be chosen so that the inequality holds.

Taking the differentiation through the integral we obtain

$$\frac{\omega T}{2\pi} = \frac{1}{2\pi \mathrm{i}} G(h) \oint^{(h+)} \frac{\mathrm{d}h'}{[h'F(h') - hF(h)]}. \tag{3.12}$$

Thus we have no singularity at $h' = 0$ and a simple pole at $h' = h$, therefore

$$\frac{\omega T}{2\pi} = G(h) \left\{ \frac{h' - h}{h'F(h') - hF(h)} \right\}_{h'=h} \tag{3.13}$$

and by taking the limit as $h' \to h$ it is a simple task to show that

$$\frac{\omega T}{2\pi} = G(h)[G(h)]^{-1} = 1. \tag{3.14}$$

4. Generalizations and conclusions

The ideas of section 3 can be extended to the general case where we are able to show that

$$\frac{\mathrm{d}x\,(y)}{\mathrm{d}y} = \left[\frac{\mathrm{d}y\,(x)}{\mathrm{d}x}\right]^{-1} \tag{4.1}$$

for any monotonically increasing function $y(x)$. By starting with the more general form of the Lagrange expansion,

$$x(y) = x_0 + = \sum_{k=1}^{\infty} \frac{(y-y_0)^k}{k!} \left[\left(\frac{\mathrm{d}}{\mathrm{d}x'}\right)^{k-1} \left\{\frac{x'}{f(x')-y_0}\right\}^k\right]_{x'=x_0} \tag{4.2}$$

where $y = f(x)$, $y_0 = f(x_0)$ and $f'(x_0) \neq 0$. It is a simple matter of following the method in the previous section to show

$$\frac{\mathrm{d}x}{\mathrm{d}y} = \frac{1}{2\pi\mathrm{i}} \oint^{(x_0+)} \sum_{\kappa=0}^{\infty} (F(x))^{\kappa} \frac{\mathrm{d}x'}{[F(x')]^{\kappa+1}} \tag{4.3}$$

where $F(x) = f(x) - y_0$. It also follows that

$$\frac{\mathrm{d}x}{\mathrm{d}y} = \frac{-1}{2\pi\mathrm{i}} \left[\frac{\mathrm{d}y}{\mathrm{d}x}\right]^{-1} \frac{\mathrm{d}}{\mathrm{d}x} \oint_{|x'|>|x|}^{(x_0+)} \ln\left[1 - \frac{F(x)}{F(x')}\right] \mathrm{d}x'. \tag{4.4}$$

This is where the restriction of the monotonicity of $F(x)$, and hence $y(x)$, arises and cannot be relaxed as in the previous case. Thus,

$$\frac{\mathrm{d}x\,(y)}{\mathrm{d}y} = \frac{1}{2\pi\mathrm{i}} \oint^{(x+)} \frac{\mathrm{d}x'}{[F(x') - F(x)]} = \left[\frac{\mathrm{d}y\,(x)}{\mathrm{d}x}\right]^{-1}. \tag{4.5}$$

In order to consider the convergence properties and analyticity domain of (2.23) and (2.25), it is necessary to use d'Alembert's ratio test and, hence, we have to be able to evaluate the nth term as $n \to \infty$. Due to the combinatorial nature of the expressions (Comtet 1974, Riordan 1958), an asymptotic form is far from evident and hence we could only check the ratio of successive terms for a range of values of α for limited values of n. By using published algorithms (Nijenhuis and Wilf 1975), we were able to generate the required partitions and calculate the ratios out as far as $n = 80$. Although clearly unacceptable as proof of convergence, the results were suggestive of a radius of convergence and hence a definite analyticity domain for each case. However, the question of convergence must remain an open question.

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