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# On the Anharmonic Oscillator

ANDREW D. BOOTH

*Institute of Ocean Sciences, P. O. Box 6000,*
*Sidney, British Columbia V8L 4B2, Canada*

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An examination of the mean-square displacement function and of a continued fraction approximation to it shows that simple approximations are available which involve only square-root functions. Comparative data are presented.

## INTRODUCTION

McLachlan and Foster [1] and Morita and Frood [2] have drawn attention to the importance of the anharmonic, mean square, displacement function

$$\langle x^2 \rangle = \frac{\int_{-\infty}^{\infty} x^2 \exp[-\beta V(x)]\, dx}{\int_{-\infty}^{\infty} \exp[-\beta V(x)]\, dx} \tag{1}$$

where $\beta = 1/kT$ and

$$V(x) = ax^2 + bx^4. \tag{2}$$

Morita and Frood have shown [2] that $\langle x^2 \rangle$ can be expressed in the form of a continued fraction

$$\langle x^2 \rangle = (1/2\beta a)\, \lambda(z) \tag{3}$$

where

$$z = b/\beta a^2 \qquad \text{and} \qquad \lambda(z) = 1/1 + 3z/1 + 5z/1 + 7z/1 + \cdots. \tag{4}$$

These authors provide a graph of $\lambda(z)$ vs $z$ which covers the range $z = 1,..., 10$. They also imply that the continued fraction (4) provides a simple method for calculating $\lambda(z)$.

While this statement is true for relatively small values of $z$, it is untrue when $z$ is appreciably greater than unity sice the continued fraction (4) converges very slowly in this region.

The purpose of this paper is to provide an asymptotic expression for $\lambda(z)$ and also to exhibit two very simple approximating functions for $\lambda(z)$ which cover the whole range $0 \leqslant z \leqslant \infty$.



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## THE ASYMPTOTIC APPROXIMATION

Making the substitution $y = x(\beta b)^{1/4}$, Eq. (1) reduces to

$$\langle x^2 \rangle = \frac{1}{\beta a \sqrt{z}} \frac{\int_0^\infty y^2 e^{-z^{-1/2}y^2} e^{-y^4}\, dy}{\int_0^\infty e^{-z^{-1/2}y^2} e^{-y^4}\, dy}$$

whence

$$\lambda(z) = \frac{2}{\sqrt{z}} \frac{\int_0^\infty y^2 e^{-z^{-1/2}y^2} e^{-y^4}\, dy}{\int_0^\infty e^{-z^{-1/2}y^2} e^{-y^4}\, dy} \tag{5}$$

Expanding $e^{-z^{-1/2}y^2}$ in powers of $y$, and using the well-known integral

$$\int_0^\infty e^{-x^q} x^p\, dx = \frac{1}{q} \Gamma\left(\frac{p+1}{q}\right)$$

Eq. (5) becomes

$$\lambda(z) = \frac{2}{\sqrt{z}} \frac{\Gamma(\frac{3}{4}) \mp \Gamma(\frac{5}{4})/\sqrt{z} + \Gamma(\frac{7}{4})/2!\, z \mp \cdots}{\Gamma(\frac{1}{4}) \mp \Gamma(\frac{3}{4})/\sqrt{z} + \Gamma(\frac{5}{4})/2!\, z \mp \cdots} \tag{6}$$

where the negative signs refer to the case where $a$ in (2) is positive while the positive signs apply for negative $a$. Thus, as $z \to \infty$,

$$\lambda(z) \to \frac{2\Gamma(\frac{3}{4})}{\Gamma(\frac{1}{4})\sqrt{z}} = \frac{0.675978}{\sqrt{z}} \tag{7}$$

Series (6) forms a convenient means of calculating accurate values of $\lambda(z)$ for $z > 1$. Three or four terms provide four place accuracy.

It is simple to extend the foregoing analysis to generate moments of order $2n$, the same procedure leads to

$$\langle x^{2n} \rangle = \frac{1}{z^{n/2}(ab)^n} \frac{\int_0^\infty y^{2n} e^{-z^{-1/2}y^2} e^{-y^4}\, dy}{\int_0^\infty e^{-z^{-1/2}y^2} e^{-y^4}\, dy}$$

and thus to

$$\langle x^{2n} \rangle = \frac{1}{z^{n/2}(ab)^n} \frac{\Gamma\left(\frac{2n+1}{4}\right) \mp \Gamma\left(\frac{2n+3}{4}\right)\sqrt{z} + \Gamma\left(\frac{2n+5}{4}\right)\Big/ 2!\, z \mp \cdots}{\Gamma(\frac{1}{4}) \mp \Gamma(\frac{3}{4})/\sqrt{z} + \Gamma(\frac{5}{4})/2!\, z \mp \cdots}$$

## Two Approximations

The limiting asymptotic form of $\lambda(z)$ provided by (7) suggests approximations of the type

$$\lambda(z) \approx \sum_{i=1}^{n} \frac{a_i}{\sqrt{z_i + \alpha_i^2}} \tag{8}$$

Two such approximations have been derived ($n = 2$ and $n = 3$). First we note that as a series the continued fraction is

$$\lambda(z) = 1 - 3z + 24z^2 - 297z^3 + 4896z^4 - 100{,}278z^5 + \cdots \tag{9}$$

For the two-term approximation we chose $a_i$, $\alpha_i$ so that

$$\lambda(0) = 1, \qquad \lambda'(0) = -3, \qquad \lambda''(0) = 48, \qquad \lambda(\infty) \to 0.675978/\sqrt{z}$$

These lead to

$$\frac{a_1}{\alpha_1} + \frac{a_2}{\alpha_2} = 1$$

$$\frac{a_1}{\alpha_1^3} + \frac{a_2}{\alpha_2^3} = 6$$

$$\frac{a_1}{\alpha_1^5} + \frac{a_2}{\alpha_2^5} = 64$$

$$a_1 + a_2 = 0.675978 \quad (= K \text{ say})$$

To solve these equations we note that

$$\frac{a_1}{\alpha_1^5} + \frac{a_2}{\alpha_2^5} = \left(\frac{a_1}{\alpha_1^3} + \frac{a_2}{\alpha_2^3}\right)\left(\frac{1}{\alpha_1^2} + \frac{1}{\alpha_2^2}\right) - \frac{1}{\alpha_1^2\alpha_2^2}\left(\frac{a_1}{\alpha_1} + \frac{a_2}{\alpha_2}\right)$$

whence

$$6\left(\frac{1}{\alpha_1^2} + \frac{1}{\alpha_2^2}\right) - \frac{1}{\alpha_1^2 \cdot \alpha_2^2} = 64 \tag{10}$$

Again,

$$\frac{a_1}{\alpha_1^3} + \frac{a_2}{\alpha_2^3} = \left(\frac{a_1}{\alpha_1} + \frac{a_2}{\alpha_2}\right)\left(\frac{1}{\alpha_1^2} + \frac{1}{\alpha_2^2}\right) - \frac{1}{\alpha_1\alpha_2}\left(\frac{a_2}{\alpha_1} + \frac{a_1}{\alpha_2}\right) \tag{11}$$

But

$$\left(\frac{1}{\alpha_1}+\frac{1}{\alpha_2}\right)(a_1+a_2)=\left(\frac{a_1}{\alpha_1}+\frac{a_2}{\alpha_2}\right)+\left(\frac{a_2}{\alpha_1}+\frac{a_1}{\alpha_2}\right)=K\left(\frac{1}{\alpha_1}+\frac{1}{\alpha_2}\right)$$

whence

$$\frac{a_2}{\alpha_1}+\frac{a_1}{\alpha_2}=K\left(\frac{1}{\alpha_1}+\frac{1}{\alpha_2}\right)-1$$

Thus, from (11),

$$\frac{1}{\alpha_1^2}+\frac{1}{\alpha_2^2}-\frac{1}{\alpha_1\alpha_2}\left[K\left(\frac{1}{\alpha_1}+\frac{1}{\alpha_2}\right)-1\right]=6 \tag{12}$$

Since

$$\frac{1}{\alpha_1^2}+\frac{1}{\alpha_2^2}=\left(\frac{1}{\alpha_1}+\frac{1}{\alpha_2}\right)^2-\frac{2}{\alpha_1\alpha_2}$$

Eqs. (10) and (12) are readily solved for $(1/\alpha_1+1/\alpha_2)$ and $1/\alpha_1\alpha_2$ and thence $\alpha_1, \alpha_2$ and $a_1, a_2$ can be determined. The result is

$$\lambda(z)\approx\frac{0.140082}{\sqrt{z+0.086573}}+\frac{0.535896}{\sqrt{z+1.046281}} \tag{13}$$

A comparison with the values calculated from the continued fraction is exhibited in Table I.

The value for $z=10$ required 961 terms of the continued fraction for four-place accuracy. That for $z=100$ required 7905 terms to produce the result as 0.06. The value given was obtained by Romberg integration using Eq. (5). This method will procude eight-place accuracy (if desired!) without difficulty.

For the three-term approximation a more sophisticated approach is needed, and the following is a sketch of a method which is applicable to any number of terms.

TABLE I

Exact and Approximated Values of $\lambda(z)$

| $\alpha$ | $z$: 0 | .0001 | .001 | .01 | .1 | 1.0 | 10 | 100 |
|---|---|---|---|---|---|---|---|---|
| Exact | 1 | .99970 | .99702 | .9721 | .818 | .470 | .189 | .066 |
| Eq. (13) | 1 | .99970 | .99702 | .9722 | .825 | .509 | .205 | .067 |
| Ex. (16) | 1 | .99970 | .99702 | .9721 | .819 | .489 | .203 | .067 |

First we note that, for the three-term case, the equations are

$$\sum_{i=1}^{3} a_i = K, \qquad \sum_{i=1}^{3} \frac{a_i}{\alpha_i^5} = \frac{2^2}{1\cdot 3}\lambda''(0) = \omega_5$$

$$\sum_{i=1}^{3} \frac{a_i}{\alpha_i} = 1 = \omega_1 \quad \text{(say)}, \qquad \sum_{i=1}^{3} \frac{a_i}{\alpha_i^7} = \frac{2}{1\cdot 3\cdot 5}\lambda^{(3)}(0) = \omega_7$$

$$\sum_{i=1}^{3} \frac{a_i}{\alpha_i^3} = 2\lambda'(0) = \omega_3, \qquad \sum_{i=1}^{3} \frac{a_i}{\alpha_i^9} = \frac{2^4}{1\cdot 3\cdot 5\cdot 7}\lambda^{(\mathrm{iv})}(0) = \omega_9$$

Assume that $1/\alpha_1^2$, $1/\alpha_2^2$, $1/\alpha_3^2$ are the roots of

$$x^3 + lx^2 + mx + n = 0 \tag{14}$$

This equation also implies

$$a_i x^{3+p} + a_i l x^{2+p} + a_i m x^{l+p} + a_i n x^p = 0$$

Whence, using the original equations,

$$\begin{aligned} \omega_9 + l\omega_7 + m\omega_5 + n\omega_3 &= 0 \\ \omega_7 + l\omega_5 + m\omega_3 + n\omega_1 &= 0 \end{aligned} \tag{15}$$

If $\omega_{-1}$ were known, a third equation would be available and the system could be solved directly to give $l$, $m$, and $n$. Equation (14) could then be solved to give $1/\alpha_1^2$, $1/\alpha_2^2$, $1/\alpha_3^2$; however, $\omega_{-1}$ is unknown.

Equation (15) can be solve to give $l$, $m$ in terms of $n$; the solution is of the form

$$l = en + f$$

$$m = gn + h$$

where $e$, $f$, $g$, and $h$ are numerical constants. These values of $l$ and $m$ are now substituted into (14) and the roots are computed for a range of negative values of $n$. Negative because all roots must be real and positive.

In practice the roots are well separated and relatively insensitive to $n$. Having computed the roots, the values of the residual

$$R = \left(\omega_9 - \sum_{i=1}^{3} \frac{a_i}{\alpha_i^9}\right)$$

are calculated for each set of roots and that set is selected which minimizes $R$. These roots are used, with the first three members of the defining set of equations, to evaluate approximate values of $a_1, a_2, a_3$, and the last step of the process is to use the six approximate values of $a_1, a_2, a_3$, $1/\alpha_1$, $1/\alpha_2$, $1/\alpha_3$ as starting values in a classical iterative procedure [3] to produce accurate values of these parameters. It turns out that, in the three-term case, only two iterations are needed to produce six-place accuracy. The result is

$$\lambda(z) \approx \frac{0.012583}{\sqrt{z+0.043935}} + \frac{0.220347}{\sqrt{z+0.135207}} + \frac{0.443048}{\sqrt{z+1.690875}} \tag{16}$$

The accuracy is somewhat better than that provided by the two-term approximation (13), the actual values being shown in the last line of Table I.

## Observations and Conclusion

It will be seen that the simple approximations involve errors of about 10% in the range $z = 1$ to 10. If these are deemed to be unacceptable, the series (6) and (9) are simple to code on a digital computer and converge with sufficient rapidity to provide high accuracy if this is wanted. Alternatively, Romberg integration applied directly to (5) is also rapidly convergent and is a good method to use if six decimal-place accuracy is wanted. Finally, it may be remarked that although the author has not had occasion to use the moment functions in further manipulations which require closed analytical forms, colleagues have stated that further operations which involve differentiations and integration are sometimes needed. In these the simple surd expressions (13) and (16) seem to offer some utility.

The same remark applies to the series (9) which gives good convergence for small values of $z$.

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## References

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