Revista Brasileira de Física, Vol. 15, nº 1, 1985

On the Efficiency of the Continued Fraction Expansion Method

B.J.O. FRANCO, A.S.T. PIRES and **A.P. SILVA**

Departamento de Física, Universidade Federal de Minas Gerais, Caixa Postal 702, Belo Horizonte, 30000, MG, Brasil

Recebido em 21 de maio de 1985

Abstract To test the efficiency of the continued fraction expansion method we start with an a priori known analytical curve $F(\omega)$, calculate the static moments and then, applying the cutoff's most used in the literature, compare the approximated curves with the original ones. We show that, except in some special cases, it is almost impossibletouse the method when only the second and fourth moments are known.

1. INTRODUCTION

The continued fraction expansion method proposed by Mori[1], where the relaxation-shape function $\psi(\omega)$ is expressed in terms of static correlation functions, is one of the most used methods in the literature, for the study of the dynamics of physical systems. In this expansion, coherent behavior is extracted at each stage of development leaving, as undetermined remainders, the Laplace transforms of memory functions. Despite its large use, the efficiency of the method is not much discussed[2]. In this paper, to test the efficiency of thecontinued fraction expansion method, we start with an a priori known analytical curve $F(\omega)$, calculate the static moments and then, applying the cut-off's most used in the literature, compare the approximated curves with the original ones.

Anologous results are found in the literature for Padé Approximants[3] but this method makes use of high order moments and in our analysis we use only lower order moments. On the other hand the equivalence between the Padé Approximant and the Continued Fraction Method Expansion is not completely established.

2. THEORY

The relaxation-shape function $\psi(z)$ can be exactly represented by the continued fraction expansion

$$\psi(z) = \frac{1}{z + \delta_1 f_1(z)}, \quad f_j(z) = \frac{1}{z + \delta_{j+1} f_{j+1}(z)}, \tag{2.1}$$

where $z = i\omega$ and $\delta_1 = M_2$, $\delta_2 = M_4/M_2 - M_2$ ..., with M_n, the n-th moment, given by

$$M_n = \langle \omega^n \rangle \equiv \int_{-\infty}^{\infty} \omega^n F(\omega)\, d\omega, \quad F(\omega) = \frac{1}{\pi} \mathrm{Re}\, [\psi(z=i\omega)] . \tag{2.2}$$

Because equation (2.1) has an infinite number of terms, in general, a cutoff must be considered. Two difficulties come about. First, in most problems, only the lower order moments can be analytically calculated. The second difficulty has to do with which function should be used to cutoff the expansion. To overcome this difficulty, a variety of approximation methods have been proposed by several authors[4-11]. These methods in general depend on both the magnitude of the available δ's and the temperature region of interest in the spectra under consideration.

The comparison of the results theoretically obtained with the experimental data does not allow a good check of the method for several reasons. Consider, for instance, the inelastic neutron scattering technique for magnetic systems. Although it gives directly the spectral function $F(\omega)$, there are problems with the convolution of experimental data and the apparatus response and also with the poor resolution around $q=0$ and $\omega=0$. Besides this, frequently the available data are in regions of spectrum where different cutoff functions (memory functions) give roughly the same results.

Another reason has to do with the Hamiltonian which may not be the right one. An example is the Ising model in a transverse field which may be appropriate for the study of the thermodynamics of ferroelectrics but may not be good for the study of its dynamics. Even if the Hamiltonian is adequate, the approximations used in the calculation of the moments (mean field approximation, random phase approximation, etc) certainly do not contribute for a tractable check.

Our investigation on the efficiency of the continued fraction expansion method proceeds as follows. We start with a known function $F(\omega)$ and calculate the lower order moments exactly. Then by using

these moments and the most common types of cutoff functions we try to reproduce the original function $F(\omega)$. It is worth mentioning that in our case the moments can all be exactly calculated in principle; however we calculate only the lower order ones because, in practical cases, only these are calculable.

The approximations considered in this paper are the so called f_∞ approximation[8], the gaussian approximation[9] and the N-pole approximation[11]. The first one consists in taking $f_{j+1}(z) = f_j(z)$, which leads to

$$f_j(z) = (-z + (z^2 + 4\delta_{j+1})^{1/2})/2\delta_{j+1} \quad . \tag{2.3}$$

The gaussian approximation consists in cutting off the expansion of $\Psi(z)$ with the furiction

$$f_j(\omega) = \frac{1}{\delta_{j+1}} \{\Gamma(\frac{\omega}{\delta_{j+1}}) - \Delta(\frac{\omega}{\delta_{j+1}})\}, \tag{2.4}$$

where

$$\Gamma(x) = (\frac{\pi}{2})^{1/2} \exp(-x^2/2) \quad ,$$

and

$$\Delta(x) = \exp(-x^2/2) \int_0^x ds \exp(s^2/2) \quad .$$

This is equivalent to cutting the expansion of the inverse Laplace transform of $f_j(w)$ through the memory function

$$f_j(t) = \exp(-t^2/2\delta_{j+1}) \quad .$$

Basically the N-pole approximation consists in replacing $f_N(\omega)$ by a constant which, in this paper, is chosen according to the Lovesey and Meserve approach[4]. The N-pole approximation is equivalent to cutting off the expansion one stage before, using an exponential function for $f_{N-1}(t)$.

The original set of functions $F(\omega)$ we work with is of three types. The first is a sum of three gaussians,

$$F(\omega) = A \exp(-\alpha\omega^2) + B \{\exp(-\gamma(\omega+\omega_0)^2 + \exp(-\gamma(\omega-\omega_0)^2)\}, \tag{2.6}$$

where A, B, a, γ and ω_0 are parameters to be varied. This is certainly an important set of functions for physical problems. By changing the parameters we can have one central peak, two lateral peaks and three peaks. The second type of functions is the Fourier transform of

$$F(t) = \exp(-at^2)\ \frac{\sin bt}{bt}\ , \tag{2.7}$$

which is important mainly in the study of F^{19} magnetic absorption lines in CaF_2 [12].

By setting b=0, $F(\omega)$ reduces to a gaussian function and by setting a=0 it reduces to the square function, a physically important function as well. The third set of functions $F(\omega)$ that we investigate is the Fourier transform of

$$F(t) = \exp(-t^{3/2})\ , \tag{2.8}$$

which gives the eletronic paramagnetic ressonance lineshape in quasi-one-dimensional rnagnetic systems in an external magnetic field paralell to the main chain[13]. We could as well have chosen the Lorentzian function to study but the N-pole approximation reproduces it correctly.

3. RESULTS

In figures 1 to 6 we show the original function $F(\omega)$ of the type described by (2.6) as well as the functions obtained through the f_∞ approximation for f_3, the gaussian approximation for f_2 and the 4--pole approximation. In figure 7 we show the Fourier transform of (2.8) and in figure 8 the Fourier transform of (2.7) . In both figures weshow the same approximations for the continued fraction as before. As we can see (fig.2) when we have only a central peak, the f_∞ approximation works reasonably well while the gaussian and the 4-pole approximation, although the most used in the literature, do poorly. When $F(\omega)$ has a side peak all approximations used fail. We could have tried higher order terminations but this would require knowledge of higher moments and these are not generally known for most problems of interest. It is clear from our work that the kind of function used in the trunction of the fraction is decisive in determining the form of the relaxation--shape function.

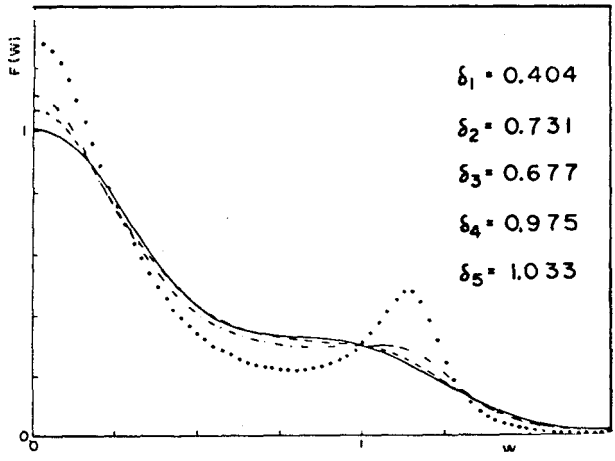

Fig.1 - ——— $F(\omega)$, Eq. (2.6) with $A=1.$, $B=.3$, $\alpha=5.$, $\gamma=5.$, $\omega_0=9$; ..... 4-pole approxirnation; ----- f_∞ approximation for $f_3(z)$; -.-.-.- gaussian approximation for $f_2(z)$.

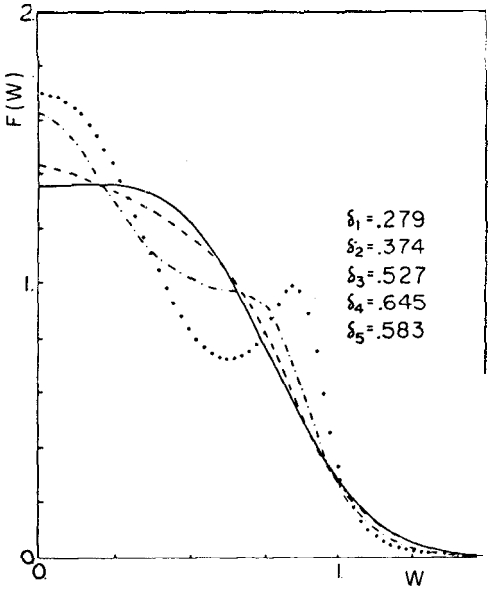

Fig.2 - ——— $F(\omega)$, Eq. (2.6) with A $=.8$, $B=1.$, $\alpha=5.$, $\gamma=5.$, $\omega_0=.5$; ..... 4-pole approximation; ----- f_∞ approximation for $f_3(z)$; -.-.-.-. gaussian approximation for $f_2(z)$.

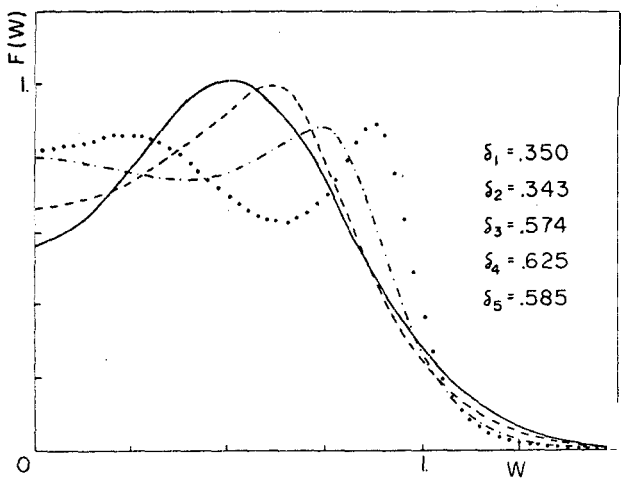

Fig. 3 - ——— $F(\omega)$, Eq. (2.6) with A=0., B=1., α=5., γ=5., ω_0=.5; ..... 4-pole approximation; ----- f_∞ approximation for $f_3(z)$; -·-·- gaussian approximation for $f_2(z)$.

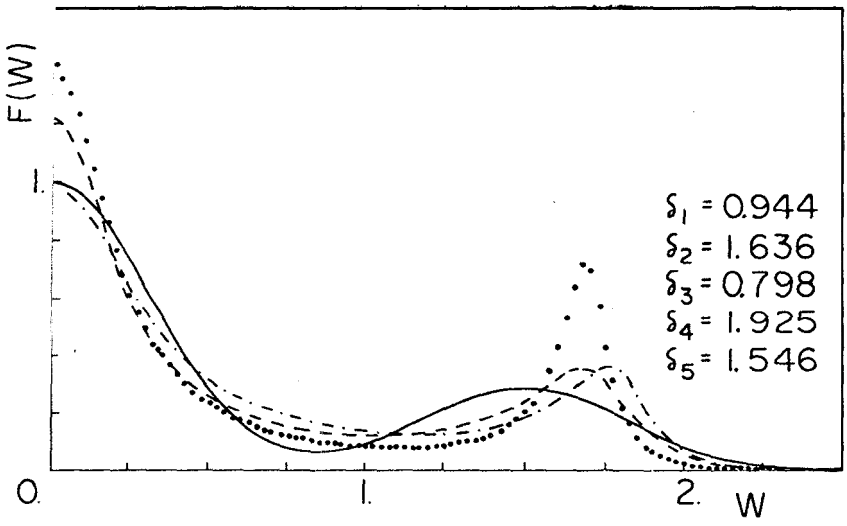

Fig. 4 - ——— $F(\omega)$, Eq. (2.6) with A=1., B=.3, α=5., γ=5., ω_0=1.5; ..... 4-pole approximation; ----- f_∞ approximation for $f_3(z)$; -.-.-.- gaussian approximation for $f_2(z)$.

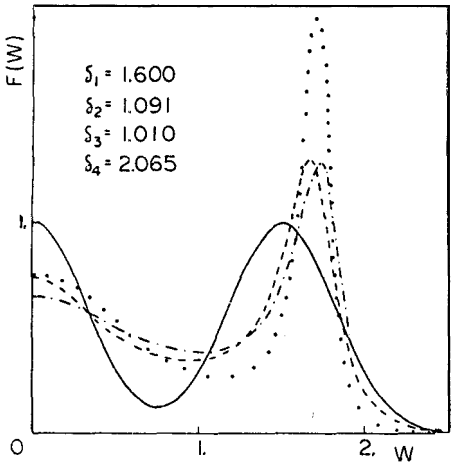

Fig.5 - ——— $F(\omega)$, Eq. (2.6) with A = 1., B = 1., α=5., γ=5., ω_0=1.5; ..... 4-pole approximation; ----- f_∞ approximation for $f_3(z)$; -.-.- gaussian approximation for $f_2(z)$.

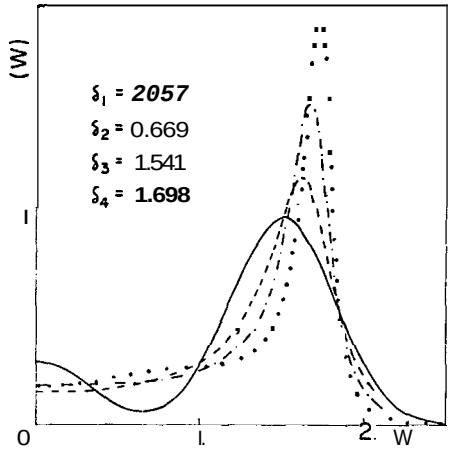

Fig.6 - ——— $F(\omega)$, Eq. (2.6) with A = .3, B = 1., α =5., γ =1.5; ..... 4-pole approximation; --- f_∞ approximation for $f_3(z)$; -.-.-.- gaussian approximation for $f_2(z)$.

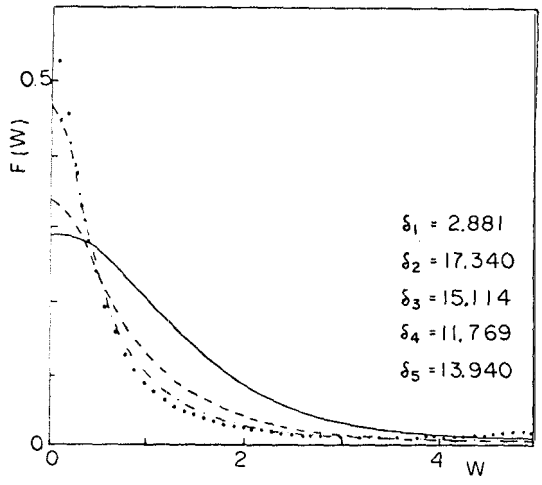

Fig.7 - —— $f(\omega)$, Eq. (2.8) ; ..... 4-pole approximation; ----- f_∞ approximation for $f_3(z)$; -.-.-.- gaussian approxirnation for for $f_2(z)$.

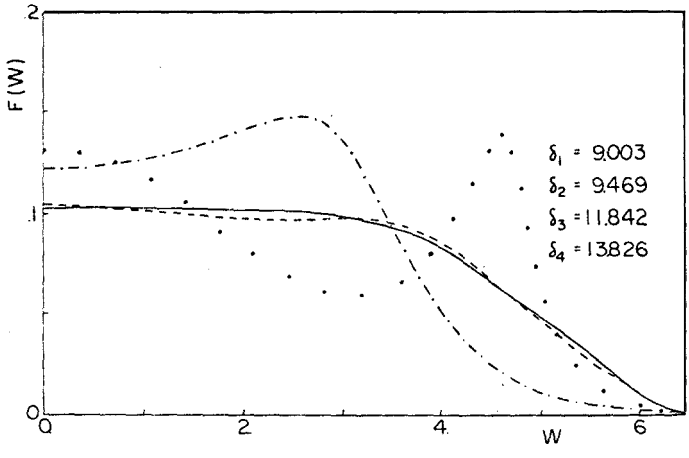

Fig. 8 - —— $F(\omega)$, Eq. (2.7); ..... 4-pole approximation; ----- f_∞ approximation for $f_3(z)$; -.-.- gaussian approximation for $f_2(z)$.

When $F(\omega)$ is a sum of N curves that are nearly Lorentzian for small ω we can show that $6_{N+1} << \delta_N$ and in this case a N-pole approximation for $F(\omega)$ works quite well. Also there are some models where the δ'_n can be cãlculated to all orders and, in these cases, the memory function can be exactly calculated[14]. In general, however, as our work shows, it is quite hard to get a good fitting using the continued fraction expansion and this becomes practically impossible when only a few 6's are known (e.g. 6, and 6) as it happens in a lot of problems in the literature[5,15,16]. We have also used other kinds of cutoff, such as gaussian approximation for $f_3(z)$, f_∞ approximation for $f_4(z)$, 5-pole approxirnation, but we have not obtained any improvement over the results preserited here. In all figures we show the corresponding values for the 6's parameters.

We are grateful to Professor B.V. Costa for colaboration in the calculations. This work was supported by CNPq and FINEP, Brasil.

REFERENCES

1. H.Mori, Progr. Theor. Phys. 34, 399 (1965).
2. M.H. Lee and R. Dekeyser, Physica, 86 - *88*B, 1273 (1977).
3. *Padé Approximants Method and its Applications to Mechanics - Lectures Notes in Physics* - Vol. 47 (Edited by H. Cabannes - Springer--Verlag) and references quoted therein.
4. S.W.Lovesey and R.A.Meserve, Phys.Rev.Lett. 28, 614 (1972); J.Phys. C: Solid St. Phys. 6, 79 (1973).
5. K. Tomita and H. Tomita, Progr. Theor. Phys. 45, 1407 (1971).
6. H. Tomita and H. Mashiyama, Progr. Theor. Phys. 48, 1133 (1972).
7. K. Tomita and H. Mashiyama, Progr. Theor. Phys. *51*, 1312 (1974).
8. U. Balucani and V. Tognetti, Sol. St. Comm. 20, 527 (1976); Phys. Lett. 60 A, 365 (1977); Phys. Rev. B*16*, 271 (1977).
9. H. de Raedt and B. de Raedt, Phys. Rev. B*15*, 5379 (1977).
10. U. Balucani, V. Tognetti and P. Valluri, Phys. Rev. A*17*, 177 (1979).
11. H. de Raedt, Phys. Rev. B*19*, 2585 (1979).
12. A. Abragarn (1961) - *The Principles of Nuclear Magnetism* (Oxford U. P. London) Chapter IV.
13. R.E.Dietz, F.R.Merrit, R.Dingle, Daniel Hone, B.G.Silbernagel, P.M.

Richards, Phys. Rev. Lett. 26, 1186 (1971).

14. M.H.Lee, Phys, Rev. B*26*, 2547 (1982).

15. T.N.Tommet and D.L.Huber, Phys. Rev. B*11*, 1971 (1975).

16. A.P.Young and B.S.Shastry, J.Phys. C*15*, 4547 (1982).

Resumo

Para testar a eficiência do método da expansão em frações continuadas considerarnos uma curva analítica $F(\omega)$ conhecida a priori, calculamos os momentos estáticos e, então, aplicando os cortes mais usados na literatura, comparamos as curvas aproximadas com a curva original. Mostramos que, exceto em alguns casos especiais, é impossível usar o método quando apenas o segundo e quarto momentos são conhecidos.