Numerical Investigation of the Friedrichs Model Dispersion Relation

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The numerical procedure of Marchand and a zero searching routine are applied to the study of the zero trajectories of the complex transcendental equation

$$\omega_0 - z - \lambda^2 \int_0^1 \frac{\phi(\omega)}{\omega - z} d\omega - 2\pi i \lambda^2 \phi(z) = 0,$$

where $\phi(\omega)$ belongs to a class of fourth degree polynomials. Such dispersion relations arise in the context of the Friedrichs model and their solution is important for theories of unstable states.

1. INTRODUCTION

The Friedrichs model [1, 2] consists of an unperturbed Hamiltonian with an absolutly continuous spectrum extending over some interval (a, b) of the real axis and a point eigenvalue ω_0 embedded in it. There is a perturbation λV , λ being a real parameter coupling the point eigenvalue to the continuum.

For our purpose it is sufficient to notice [3] that the possible point eigenvalues of this Hamiltonian are given by the zeros of a function of the form

$$\eta(z) = \omega_0 - z - \lambda^2 \int_a^b d\omega \, \frac{\phi(\omega)}{\omega - z} \,, \tag{1.1}$$

where

$$\begin{aligned} \phi(a) &= \phi(b) = 0, \\ \phi(\omega) &> 0 \qquad (a < \omega < b). \end{aligned}$$

This function $\eta(z)$ is analytic in the complex plane except for a cut along (a, b). Depending on λ^2 it may have none, one or two (real) zeros. In fact if

$$\lambda_{I}^{2} = \min\left\{ (\omega_{0} - a) \left[\int_{a}^{b} d\omega \frac{\phi(\omega)}{\omega - a} \right]^{-1}, \ (\omega_{0} - b) \left[\int_{a}^{b} d\omega \frac{\phi(\omega)}{\omega - b} \right]^{-1} \right\}$$
(1.3a)

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and

$$\lambda_{II}^{2} = \max\left\{ (\omega_{0} - a) \left[\int_{a}^{b} d\omega \frac{\phi(\omega)}{\omega - a} \right]^{-1}, \ (\omega_{0} - b) \left[\int_{a}^{b} d\omega \frac{\phi(\omega)}{\omega - b} \right]^{-1} \right\}, \quad (1.3b)$$

then for

$$\begin{array}{c} \lambda^2 < \lambda_I^2 \\ \lambda_I^2 < \lambda^2 < \lambda_{II}^2 \\ \lambda_{II}^2 < \lambda^2 \end{array} \end{pmatrix} H \text{ has } \left\{ \begin{array}{c} \text{no} \\ \text{one} \\ \text{two} \end{array} \right\} \text{ point eigenvalue(s).}$$

Note that because of (2) the eigenvalues of H, if any, lie outside the interval (a, b).

According to the previous remarks the eigenvalue ω_0 of H "disappears" because of the perturbation, provided that λ^2 is sufficiently small. However, a trace of this eigenvalue may be found as a zero of the analytic continuation of $\eta(z)$. The knowledge of the behavior of these zeros is important in theories of unstable states [4, 10, 11]. If $\phi(z)$ is analytic in some region near the cut the analytic continuation of $\eta(z)$ crossing the cut from above (below) is given by

$$\eta^{\pm}(z) = \omega_0 - z - \lambda^2 \int_a^b d\omega \, \frac{\phi(\omega)}{\omega - z} \mp 2\pi i \lambda^2 \phi(z). \tag{1.4}$$

As the interval (a, b) is finite we may write $\eta(z)$ in the form

$$\eta(z) = \omega_0 - z - \lambda^2 \int_a^b d\omega \, \frac{\phi(\omega) - \phi(z)}{\omega - z} - \lambda^2 \phi(z) \log \left(\frac{z - b}{z - a}\right) \tag{1.5}$$

and the question of analytic continuation reduces to that of the choice of the correct branch for the logarithm.

We remark that for a given ω_0 the two critical values from (3), λ_I^2 and λ_{II}^2 , are as a rule different, but a specific $\bar{\omega}_0$ can always be found so these two values coalesce. From $\lambda_I^2 = \lambda_{II}^2 = \lambda_D^2$ and making

$$\alpha(x)=\int_a^b d\omega\,\frac{\phi(\omega)}{\omega-x}\,,$$

we have

$$\lambda_D^2 = \frac{\bar{\omega}_0 - a}{\alpha(a)} = \frac{\bar{\omega}_0 - b}{\alpha(b)},$$

$$\bar{\omega}_0 = \frac{b - a\alpha(b)/\alpha(a)}{1 - \alpha(b)/\alpha(a)},$$
(1.6)

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and

$$\lambda_D^2 = \left[\int_a^b d\omega \ u(\omega)\right]^{-1},\tag{1.7}$$

where

$$u(\omega) = -\phi(\omega)[(\omega - a)(\omega - b)]^{-1}$$
(1.8)

As $\alpha(b)/\alpha(a)$ is essentially a negative quantity, $a < \bar{\omega}_0 < b$.

Considering now the two principal branches of $\eta(z)$ which we obtain by analytic continuation we notice it is sufficient to study the roots of one of them. From the principle of reflection it follows that $\overline{\eta^+(z)} = \eta^-(\overline{z}) = 0$ and this leads to symmetrical solutions in relation to the real axis.

We expect analyticity in λ for the roots of $\eta(z)$ as functions of this parameter so they should generate a set of trajectories on the complex z plane. How many trajectories exist is dependent on determining the number of roots present for each λ^2 . To find the precise number of roots of an equation on the complex plane is an involved process. One has to depend on the explicit use of Cauchy's theorem and work through numerical contour integrations [5, 6]. Still in our problem we could limit the number of trajectories which possibly exist. Two of them attain the cut end-points for the two critical values of λ^2 . Another originates at the point ω_0 which is a solution of the uncoupled equation. Other trajectories will be associated with singular points of the density function $\phi(z)$. It is of course possible for a single curve to pass through several of these points; for instance, the trajectory coming from ω_0 can connect with one of the cut end-points.

In this paper we will present some results, mainly numerical, concerning the roots of $\eta^+(z)$ where for $\phi(\omega)$ we take a quartic polynomial, the interval of integration being (0, 1).

2. Two Numerical Methods

One possible way to deal with an equation of the type we consider is to separate it into real and imaginary parts and study the equivalent system of equations. Namely

$$\begin{cases} \text{Re } \eta^+(x, y, \lambda^2, \omega_0) = 0, \\ \text{Im } \eta^+(x, y, \lambda^2) = 0. \end{cases}$$
 (2.1)

Each equation represents a family of curves in the xy plane parametrized by λ^2 , ω_0 being fixed. The intersections of these curves which correspond to common values of λ^2 are then the solutions of the system. Such a type of approach was suggested by Marchand [4].

A computer program was employed to generate plots of the intersections with the plane x = y = 0 of the three-dimensional surfaces from (1). To λ^2 a set of values was attributed. Contour plotting routines have recently been used with satisfactory results in problems of a similar type [7, 8]. This technique affords reasonable precision when compared to iterative procedures. We have also the convenience of showing the behavior of the two parts of the dispersion relation versus the coupling constant. As the equation for the imaginary part is independent of ω_0 , the problem is simpler and we obtain immediately a representation for the λ^2 -isolines. However, this method tends to be slow in the computer and a more efficient one was envisaged.

Numerical computation was done directly in complex arithmetic and an adequate form of Muller's iteration [9] served as a zero scarching routine. The program is an elaboration of MULROOT from the CDC VIM Program Library and was written in FORTRAN. We worked in terms of an imposed bound on the modulus of $\eta^+(z)$ below which z is assumed to be a zero, local deflation being then done throughout. Solutions found for a given value of λ^2 were then reused as starting values in the next iteration. In the CDC 6400 computer we used, for a given density function, a specific value of ω_0 and a large enough number of λ^2 values so as to get sufficient definition for plotting, results were obtained in time of order 30 sec. With the first method this number increased by a factor of ten, being exclusive of off-line plot time.

3. A SAMPLE CASE: A CLASS OF QUARTIC POLYNOMIALS AS DENSITY FUNCTIONS

3.1. The form of $\phi(\omega)$

We were interested in studying a case where the function $\phi(\omega)$ should possess some generality. Initially, polynomials were chosen so that the integration in $\eta(z)$ could always be carried out explicitly. The degree of those polynomials was fixed attending to the requirement of obtaining (by a change in their coefficients) functions that in the interval in consideration should either be symmetric in relation to an axis or not, have more than one maximum or not and eventually vanish at an interior point. Essentially, the members of the class should be identified by a parameter varying in a given range so that a small change in the form of $\phi(\omega)$ could be obtained in a continuous way.

When polynomials of degree four are taken, and the interval of integration (a, b) is chosen to be (0, 1), conditions (1.2) lead to the following type of density functions,

$$\phi(\omega) = -\omega(\omega - 1) C(\omega^2 - 2F\omega + F^2 + B^2), \qquad (3.1)$$

with C a positive constant and $0 \le F \le (F + B)^{1/2}$. There is always an extremum

for $\omega = (F^2 + B^2)^{1/2}$. Keeping this quantity fixed, the occurrence of other points of stationarity depends simply on F, a form factor for $\phi(\omega)$. To attribute $(F^2 + B^2)^{1/2}$ equally distant values from the interval end-points leads to symmetrical results in relation to the axis $x = \frac{1}{2}$. Computation was performed for $(F^2 + B^2)^{1/2} = \frac{2}{3}$, a situation from which the behavior for other values of this constant can easily be inferred.

It is convenient, and is without loss of generality, to impose a condition on C so that with $u(\omega)$ defined by (1.8) we have

$$\int_0^1 d\omega \ u(\omega) = 1, \tag{3.2}$$

which leads to $C = (F^2 + B^2 - F + \frac{1}{3})^{-1}$. From (1.7) we get then $\lambda_D^2 = 1$. This is simply done to scale the range of λ^2 for the different density functions. Making λ_D^2 equal to unity ensures that the two critical λ^2 also quantities of this order.

3.2. The roots of $\eta^+(z)$

From the general form of $\eta(z)$ and (1) we write

$$\eta(z) = \omega_0 - z + \lambda^2 \int_0^1 d\omega \, \frac{\omega(\omega - 1) \, C(\omega^2 - 2F\omega + F^2 + B^2)}{\omega - z}$$

or

$$\eta(z) = \omega_0 - z + \lambda^2 \int_0^1 d\omega \, \frac{P_1 \omega^4 + P_2 \omega^2 + P_3 \omega^2 + P_4 \omega}{\omega - z} \,, \tag{3.3}$$

with

$$P_1 = C,$$

$$P_2 = -C(2F + 1),$$

$$P_3 = C(2F + F^2 + B^2),$$

$$P_4 = -C(F^2 + B^2).$$

This yields

$$\eta(z) = \omega_0 - z + \lambda^2 \left[Q_1 z^3 + Q_2 z^2 + Q_3 z + Q_4 + (P_1 z^4 + P_2 z^3 + P_3 z^2 + P_4 z) \log\left(\frac{z-1}{z}\right) \right], \qquad (3.5)$$

where

$$Q_{1} = P_{1},$$

$$Q_{2} = (\frac{1}{2}P_{1} + P_{2}),$$

$$Q_{3} = (\frac{1}{3}P_{1} + \frac{1}{2}P_{2} + P_{3}),$$

$$Q_{4} = (\frac{1}{4}P_{1} + \frac{1}{3}P_{2} + \frac{1}{2}P_{3} + P_{4}).$$
(3.6)



FIG. 1. Quartic density functions of the form $\phi(\omega) = -\omega(\omega - 1) C (\omega^2 - 2F\omega + F^2 + B^2)$ with $(F^2 + B^2)^{1/2} = 2/3$ and $C = (7/9 - F)^{-1}$, lettering scheme defined for the set of increasing values of F = 0, 5/18, $(4\sqrt{6} - 1)/18$, 33/54, 2/3.



FIG. 2. Zero trajectories of $\eta^+(z, \omega_0, \lambda^2)$ with function $A, F = 0, -1/6 \le \omega_0 \le 7/6, \omega_0 = W_i$.



FIG. 3. Zero trajectories of $\eta^+(z, \omega_0, \lambda^2)$ with function $C, F = (4\sqrt{6}-1)/18, -1/6 \le \omega_0 \le 7/6, \omega_0 = W_i$.



FIG. 4. Zero trajectories of $\eta^+(z, \omega_0, \lambda^2)$ with function $E, F = 2/3, -1/6 \le \omega_0 \le 7/6, \omega_0 = W_i$.

After (1.5) we indicate how $\eta^+(z)$ is obtained from $\eta(z)$ by a change in the position of the cut. The argument of the logarithm was chosen accordingly in the expression above, namely in the interval $(\pi, 2\pi)$, and this was then the form used for effecting numerical calculations.

For a series of values of F producing the functions depictured in Fig. 1, plots of the respective zero trajectories were obtained for various choices of the point ω_0 . Fig. 2-4 give the trajectories found for some of these density functions.

There are two trajectories, each of which attains an interval end-point for the two critical values of λ^2 . In general it can be said that if ω_0 is sufficiently near to 0 or 1 the curve starting there passes through one of these points. A third one converges with increasing λ^2 to the respective solution of $\lim_{\lambda^2 \to \infty} \eta^+(z, \lambda^2) = 0$, which exists for the class of functions considered. The curve generated by this solution with F as a parameter is given in Fig. 5.



FIG. 5. Zero trajectories of $\eta^+(z, \omega_0, \lambda^2)$ with functions A to E, $\omega_0 = W_4$. Broken line represents the trajectory of $\eta^+(z, \omega_0, \lambda^2)$ when $\lambda^2 \to \infty$, parameter F.

The set of the possible functions $\phi(\omega)$ falls into two distinct groups depending on whether there are one or two maxima in the interval (0, 1). We have examined the case of the limiting curve which lies between the two groups and has a single maximum and a point of inflexion, $F = (4\sqrt{6} - 1)/18$. These are the results shown in Fig. 3. The trajectories approach a symmetrical disposition but nothing exceptional occurs.

In the two extreme cases we study, for values of F equal to 0 and $\frac{2}{3}$, particular situations arise. For F = 0 no matter which value is taken for ω_0 the trajectory that originates there passes through one of the cut end-points. This behavior is simpler than that displayed in the more general case. For $F = \frac{2}{3}$ and if $\omega_0 \leq \frac{2}{3}$ one of them always attains the real axis at $x = \frac{2}{3}$, a point where the corresponding function $\phi(z)$ also vanishes. From (1.4) this can easily be verified.



FIG. 6. Real and imaginary parts of $\eta^+(z, \omega_0, \lambda^2) = 0$, solid and broken lines respectively, for function A, F = 0, and $\omega_0 = W_5$. Solutions occur at the intersections of the curves for the same value of λ^2 .

Figure 5 resumes the results when ω_0 is kept fixed and the function $\phi(\omega)$ changes. We show in Fig. 6 an example of the computer plots we obtained when the first method described is used.

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4. CONCLUDING REMARKS

It can be said that three trajectories exist for each of the density functions considered. The one coming from ω_0 either goes to one of the interval end-points or not, depending on the value of ω_0 . If not it converges to the respective solution of $\lim_{\lambda^2 \to \infty} \eta^+(z, \lambda^2) = 0$.

We are aware that the study made here with quartic functions presents little generality from the point of view of which type of solutions could be expected for nonpolynomial or even polynomial density functions. To compare with the quadratic case [12], the situation differs in an important aspect from the present one. There, a trajectory from ω_0 always attains a cut end-point along a continuous curve. This evidently relates to the absence of solutions for the equation we get from $\lim_{\lambda^2 \to \infty} \eta^+(z, \lambda^2) = 0$, a condition which does not hold in general.

The method we used can without undue complication be applied to other problems. So far $\phi(\omega)$ is such that the Cauchy integral can be performed explicitly this is a convenient simplification. Otherwise, we have to resort to the expression given by (1.5) and proceed by numerical quadrature, having then also to study the stability of the solutions in relation to the approximation made for the integral.

Some few properties of the zeros can also be inferred by analytic methods, and this will be the object of a forthcoming publication.

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