

THEORY OF ANALYTIC CONTINUATION AND APPLICATION TO DYNAMICAL SYSTEMS

By

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Dedication

To my parents

To my husband ,
relatives and colleagues,
without their support and
encouragement it would
have been impossible for
me to proceed.

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Abstract (II)

The first part of the dissertation is a study of the theory of analytic continuation (A.C) of function of complex variable. Theorems and examples are given to investigate the topics of direct (A.C), (A.C) along a curve, global analytic branch points, Riemann surfaces and their construction.

The second part is devoted to application of (A.C) in some problems of quantum mechanics. The generalized classical treatment of Langevin equation for a linear oscillator embedded in a bath of harmonic oscillators is solved to measure rate of energy absorption from an external radiation source. Quantum treatment applies (A.C) on the displacement imaginary-time to obtain the real-time correlation. A brief description of the implementation of the maximum entropy inversion method is given. Singular value decomposition method and numerical path integral Monte-Carlo simulation are used to get numerical solution of the same problems above.

Finally curves obtained by Fourier integrals (using A.C theory) are compared with curves obtained numerically (using statistical and simulation methods).

Introduction

- 1) in chapter 2 and 3 quantum dynamic is stimulated by performing a numerical analytic continuation of imaginary time – correlation functions.
- 2) The time – correlation function calculated along the imaginary time axis can be uniquely analytically continued to the real – time axis .
- 3) In this approach the total system is divided into a subsystem and a bath .
- 4) The effect of the bath on the system is treated perturbatively through bath time – correlation function .
- 5) The purpose of the present study is to examine the performance of the maximum entropy (ME) and singular value decomposition (SVD) analytic continuation methods to the problem of quantum mechanical vibrational relaxation.
- 6) Complicated atomic and molecular systems can be approximated very well by harmonic baths .
- 7) The one- dimensional oscillator coupled to a harmonic bath is a prototype model for studying vibrational relaxation in condensed phases .

1.1- Model system

Let us consider an oscillator linearly coupled to a bath of harmonic oscillators . the Hamiltonian of the system is

$$H = H_{\text{osc}} + H_{\text{bath}} + V_{\text{int}}$$

خلاصة البحث

الجزء الأول من الرسالة يحتوي دراسة نظرية الامتداد التحليلي (أ.ت) للدوال في متغير مركب ، اعطي عدد من النظريات والامثلة لتوضيح مواضيع في الامتداد التحليلي المباشر ، (أ.ت) علي منحنى ، نقاط التفرع في التحليل الشامل ، سطوح ريمان وانشائها .

الجزء الثاني مخصص لتطبيقات (أ.ت) في بعض مسائل ميكانيكا الكم .

تم حل معادلة لانقن بمعالجة تقليدية عامة لقياس معدل امتصاص الطاقة من مصدر اشعاع خارجي .تم تطبيق (أ.ت) علي الزمن التخيلي للازاحة لايجاد الزمن الحقيقي للازاحة اعطي وصف موجز لاعمال طريقة الاقلاب الاعظمي للانثروبي . استخدمت طريقة تفكيك القيمة المنفردة و طريقة محاكاة مونت كارلو للتكامل العددي الخطي لايجاد الحلول العددية لنفس المسائل اعلاه .

أخيرا أعطيت مقارنة المنحنيات التي تم الحصول عليها باستخدام تكاملات فورير ونظرية (أ.ت) مع المنحنيات التي تم الحصول عليها عدديا باستخدام الطرق الإحصائية وطرق المحاكاة.

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Example:

1.11 The analytical Continuation of Stieltjes's function:

The function $F(z)$ defined in $|\operatorname{ph} z| < \pi$ by equation

$$F(z) = \int_0^{\infty} e^{-s} \frac{ds}{z+s}.$$

Is the Principal branch of the confluent hypergeometric function $\psi(I, I; z)$ which has a logarithmic branch point at the origin.

Other branches can be obtained by analytical continuation in the following way.

When $R(z) > 0$ rotation of the path integration through a right angle gives the integral

$$F_1(z) = \int_0^{\infty} e^{-it} \frac{idt}{it+z} \quad (17)$$

As an alternative representation of $f(z)$ in the right hand half plane.

But $F_1(z)$ is an analytic function, regular in

$|z| > 0, -\frac{1}{2}\pi < \operatorname{ph} z < \frac{3}{2}\pi$, since the integral in (17) converge uniformly on any compact set in this sector.

Thus while $F(z)$ and $F_1(z)$ are the same function in

$-\frac{1}{2}\pi < \operatorname{ph} z < \pi$, $F_1(z)$ provide the analytical continuation of $F(z)$ across the cut $\operatorname{ph} z = \pi$.

In the third quadrant, $F(z)$ and $F_1(z)$ are different functions.

$$\begin{aligned} \text{For } F(z) - F_1(z) &= \int_0^{\infty} e^{-s} \frac{ds}{z+s} - \int_0^{\infty} e^{-it} \frac{idt}{z+it} \\ &= \lim_{R \rightarrow \infty} \int_C e^{-\sigma} \frac{d\sigma}{z+\sigma} \end{aligned} \quad (18)$$

Where c is a boundary of the quadrant $|\sigma| \leq R$, $0 \leq \arg \sigma \leq 1/2 \pi$ in the complex σ plane. When z is in the third quadrant, the pole

$\sigma = -z$ lies inside c when $R > |z|$ and so

$$F(z) - F_1(z) = 2\pi i e^z.$$

$$\text{Thus } F_1(z) = F(z) - 2\pi i e^z. \quad (19)$$

Connect the two branches in the third quadrant. Although $F(z)$ is discontinuous across the negative real axis, $F_1(z)$ is continuous, and hence, if $a > 0$,

$$F(-a+io) - F(-a-io) = -2\pi i e^{-a}$$

Stieltjes observed that both these limiting values can be expressed in terms of a Cauchy principal value integral.

For if $a > 0$ and if c is the contour of (17) indented upwards at $\sigma = a$, we have

$$\lim_{R \rightarrow \infty} \int_{c_R} e^{-\sigma} \overline{\sigma - a} d\sigma = 0$$

This gives

$$0 = \text{P} \int_0^\infty e^{-s} \frac{ds}{s-a} - \pi i e^{-a} - \int_0^\infty e^{-it} \frac{idt}{it-a}$$

or

$$F_1(-a) = \text{P} \int_0^\infty e^{-s} \frac{ds}{s-a} - \pi i e^{-a} \quad (20)$$

$$\text{Since } F(-a + io) = F_1(-a)$$

It follows that

$$F(-a - io) = \text{P} \int_0^\infty e^{-s} \overline{\frac{ds}{s-a}} - \pi i e^{-a}. \quad (21)$$

The asymptotic expansion of $F_1(z)$ can be obtained at once from (17) by integration by parts. The result is that

$$E_1(z) = \sum (-1)^{k-1} \frac{(k-1)!}{z^k}$$

as $|z| \rightarrow \infty$ in $-\frac{1}{2}\pi + \delta \leq \arg z \leq \frac{3}{2}\pi - \delta < \frac{3}{2}\pi$.

Hence, by (20)

$$\int_0^\infty e^{-s} \frac{ds}{s-a} \sim \sum_{k=1}^\infty \frac{(k-1)!}{a^k} \quad (22)$$

\rightarrow

as $a \rightarrow +\infty$ the term involving e^{-a} being omitted since it is very small compared with any terms of the series (22).

The asymptotic expansion (22) is a series of positive terms makes it more difficult to estimate the best approximation, which can be made by taking partial sums.