BRÅKET

Information om seminarier och högre undervisning i matematiska ämnen i Stockholmsområdet

NR 41 **FREDAGEN DEN 15 DECEMBER 2000**

BRÅKET

Veckobladet från Institutionen för matematik vid Kungl Tekniska Högskolan och Matematiska institutionen vid Stockholms universitet

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Sista manustid för nästa nummer: Torsdagen den 4 januari kl. 13.00.

Kurs

Dževad Belkić: The Principle and Methods of Quantum Scattering Theory / continued (The Padé-Lanczos Algorithm). Se sid. 5 – 16.

God Jul och Gott Nytt År

önskas Bråkets läsare. Nästa nummer av Bråket utkommer fredagen den 5 januari 2001.

Money, jobs: Se sidorna 3 – 5.

SEMINARIER

Fr 12–15 kl. 9.00 – 10.00. Kollokvium i fysik. Professor emeritus Bengt Nagel, Teoretisk fysik, KTH: *The quantum theory 100 years.* Sal F 01, Fysiska institutionen, KTH, Lindstedtsvägen 24, b.v. Se Bråket nr 40 sidan 6.

Fr 12–15 kl. 11.00 – 12.00. Optimization and Systems Theory Seminar. Andreas Wächter, Department of Chemical Engineering, Carnegie Mellon University, Pittsburgh, USA: *An interior point algorithm for large-scale nonlinear programming.* Seminarierum 3721, Institutionen för matematik, KTH, Lindstedtsvägen 25, plan 7. Se Bråket nr 40 sidan 5.

Fr 12–15 kl. 13.15 – 15.00. Matematikdagar 00/01. Lasse Svensson och **Ambjörn Naeve:** *Geometrisk algebra och projektiv geometri.* Sal D3, KTH, Lindstedtsvägen 5, b.v. Se Bråket nr 39 sidan 4.

Må 12–18 kl. 13.00. Licentiatseminarium i statistik. *(Observera dagen och lokalen!)* **Jan Hagberg** framlägger sin licentiatavhandling: *Centrality Testing and Distribution of the Degree Variance in Bernoulli Graphs.* Opponent: **Fil. dr Martin Karlberg,** AstraZeneca, Södertälje. Sal F 420, Södra huset, Frescati, Universitetsvägen 10 F, 4 vån. Se Bråket nr 40 sidan 7.

Må 12–18 kl. 13.15 – 14.00. Seminarium i numerisk analys. Dimitry Sokoloff, Uppsala universitet: *Alignment is a shell model of MHD turbulence.* Sal 4523, NADA, KTH, Lindstedtsvägen 3. Se Bråket nr 40 sidan 7.

Fortsättning på nästa sida.

Disputation i matematik

Anders Karlsson disputerar på avhandlingen *Semicontractions, nonpositive curvature, and multiplicative ergodic theory* fredagen den 15 december kl. 13.00 i sal E1, KTH, Lindstedtsvägen 3, b.v. Se Bråket nr 39 sidan 7.

Seminarier (fortsättning)

Må 12–18 kl. 13.15 – 15.00. Algebra and Geometry Seminar. Ralf Fröberg: *Equivalences for plane curves.* Rum 306, hus 6, Matematiska institutionen, SU, Kräftriket, Roslagsvägen 101. Se nedan.

Må 12–18 kl. 14.00 – 15.00. Presentation av examensarbete i matematik. Fredrik Stenberg: *Inverse scattering problems on graphs.* Sal 16, hus 5, Matematiska institutionen, SU, Kräftriket, Roslagsvägen 101.

Må 12–18 kl. 15.15. Seminarium i matematisk statistik. Professor Timo Koski, Matematisk statistik, Linköpings tekniska högskola: *EM-algoritmens egenskaper i beräkningsbiologi och i tillämpningar på modellbaserad klustring.* Seminarierum 3733, Institutionen för matematik, KTH, Lindstedtsvägen 25, plan 7. Se Bråket nr 40 sidan 6.

Ti 12–19 kl. 12.15 – 13.00. Presentation av examensarbete i matematik. Hillevi Gavel: *Permutationsordningar och relationsmatriser.* Sal D31, KTH, Lindstedtsvägen 17, b.v. Se Bråket nr 40 sidan 5.

On 12–20 kl. 13.15. Seminarium i analys och dynamiska system. Mattias Dahl, Hamburg: *Surgery and the spectrum of the Dirac operator.* Seminarierum 3721, Institutionen för matematik, KTH, Lindstedtsvägen 25, plan 7. Se sidan 3.

On 12–20 kl. 15.15. Presentation av examensarbete i matematisk statistik. Sotiris Tserepis: *Comparative study of expense loadings for the prospective and retrospective reserves.* Rum 306, Cramérrummet, hus 6, Matematiska institutionen, SU, Kräftriket, Roslagsvägen 101. Se sidan 3.

ALGEBRA AND GEOMETRY SEMINAR

Ralf Fröberg:
Equivalences for plane curves

Abstract: An analytic plane curve branch through the origin in $\mathbf{C}^2$ is a power series $f(X,Y) \in \mathbf{C}[[X,Y]]$ such that:

1) It is convergent in some neighbourhood of the origin and $f(0,0) = 0$ and
2) $f(X,Y)$ is irreducible in $\mathbf{C}[[X,Y]]$.

Let C and D be two analytic plane curve branches with singularities in the origin. The singularities are said to be analytically equivalent if there are open neighbourhoods U and U' of the origin in $\mathbf{C}^2$ and an analytic isomorphism $T\colon U \longrightarrow U'$ such that $T(C \cap U) = D \cap U'$. Let $C', C'', \ldots$ ($D', D'', \ldots$, resp.) be the successive quadratic transforms of C (D, resp.) when blowing up the singularity in the origin, and let e_i (e'_i, resp.) be the multiplicity of $C^{(i)}$ ($D^{(i)}$, resp.). Zariski showed that C and D are analytically equivalent if and only if $(e_0, e_1, \ldots) = (e'_0, e'_1, \ldots)$. (This is now called (a)-equivalence.) He also showed that C and D are (a)-equivalent if and only if they have the same semigroup of values. Using a lemma by Apery, we will give a very short proof of the fact that C and D are (a)-equivalent if and only if they have the same semigroups of values. All concepts are elementary and will be explained.

Tid och plats: Måndagen den 18 december kl. 13.15 – 15.00 i rum 306, hus 6, Matematiska institutionen, SU, Kräftriket, Roslagsvägen 101.

SEMINARIUM I ANALYS OCH DYNAMISKA SYSTEM

Mattias Dahl:
Surgery and the spectrum of the Dirac operator

Abstract: The Dirac operator D on a Riemannian spin manifold is a natural first order elliptic differential operator; on a compact manifold it has a discrete spectrum.

Doing surgery on a manifold is a way of changing its topology: Remove an embedded copy of $S^k \times D^{n-k}$ and glue in a copy of $D^{k+1} \times S^{n-k-1}$ — these pieces have the same boundary $S^k \times S^{n-k-1}$. This is surgery in codimension $n-k$.

I will show that surgery need not change the spectrum of D much. Given a Riemannian metric g on a compact manifold and numbers $N, \epsilon > 0$, one can carefully construct a metric $\bar{g}$ on the manifold after surgery such that the first N eigenvalues of D_g and $D_{\bar{g}}$ pairwise differ at most by ϵ. This if the codimension of the surgery is at least three. As an application I will prove that under different assumptions on the topology of the manifold one has $\dim \ker D = |\mathrm{ind}\,(D)|$ for a generic Riemannian metric. The point here is that one side of this identity is a topological invariant while the other is not.

Tid och plats: Onsdagen den 20 december kl. 13.15 i seminarierum 3721, Institutionen för matematik, KTH, Lindstedtsvägen 25, plan 7.

PRESENTATION AV EXAMENSARBETE I MATEMATISK STATISTIK

Sotiris Tserepis:
Comparative study of expense loadings for the prospective and retrospective reserves

Abstract: Insurance policyholders pay single or yearly premiums and in return the insurer provides insurance cover. This paper studies the methods that insurance companies use to cover the cost of its business. The methods for the loading of premium, mortality and interest rate are described. Further analyses and a comparison of the expense loading for the prospective and retrospective reserves in life insurance are carried out.

Tid och plats: Onsdagen den 20 december kl. 15.15 i rum 306, Cramérrummet, hus 6, Matematiska institutionen, SU, Kräftriket, Roslagsvägen 101.

MONEY, JOBS

Columnist: Pär Holm, Department of Mathematics, SU. E-mail: pho@matematik.su.se.

Info = information. This will be given and repeated until obsolete. Rely on other sources as well.
BBKTH = Bulletin Board at the Department of Mathematics, KTH.
BBSU = Bulletin Board at the Department of Mathematics, SU.
Unless stated otherwise, a given date is the last date (e.g. for applications), and the year is 2000. A number without an explanation is a telephone number.

Standard information channels

1. A channel to information from TFR: http://www.tfr.se.
2. A channel to information from NFR: http://www.nfr.se.
3. A channel to information from the European Mathematical Society: http://www.emis.de.
4. A channel to information from the American Mathematical Society: http://www.ams.org.
5. KTH site for information on funds, etc., weekly: http://www.kth.se/aktuellt/stipendier/.
6. Stockholm University site for information on funds: http://apple.datakom.su.se/stipendier/.

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7. Umeå site for information on funds: http://www.umu.se/umu/aktuellt/stipendier_fond_anslag.html.
8. Job announcement site: http://www.maths.lth.se/nordic/Euro-Math-Job.html. This is run by the European Mathematical Society.
9. KTH site for information on research: http://www.admin.kth.se/CA/extrel/index/forsk.html.

New information

Money, to apply for

10. Kungl. Vetenskapsakademien (KVA) kommer att, med ekonomiskt stöd från Knut och Alice Wallenbergs stiftelse, inrätta sju eller åtta femåriga forskartjänster. Forskartjänsterna är konstruerade så att akademien ansvarar för forskarnas anställning, medan de utför själva forskningen vid sina lärosäten som tidigare. Sista ansökningsdag är 1 februari 2001. Info: Astrid Auraldsson, 08-673 96 19, astrid@kva.se. Web-info: http://www.kva.se/sve/pg/forskning/index.asp.

Jobs, to apply for

11. Institutionen för numerisk analys och datalogi (NADA), gemensam för SU och KTH, söker för anställning vid SU en professor i datalogi med inriktning mot naturvetenskapliga tillämpningar, 22 januari 2001. Info: Ingrid Melinder, 08-790 77 98, melinder@nada.kth.se. Web-info: http://www.insidan.su.se/ledigatjanster.php3?jobb=111.

Old information

Money, to apply for

12. Kungl. Vetenskapsakademien (KVA) utlyser medel från stiftelsen G. S. Magnusons fond; till doktorander utdelas stipendier med ett engångsbelopp på normalt 7 000 kr, och till forskare som avlagt doktorsexamen 1995 eller senare utdelas forskningsanslag med i normalfallet 30 000 kr (0 – 3 år efter disputation), respektive 50 000 kr (4 – 6 år efter disputation). Utöver detta finns även medel avsedda speciellt för stöd till svenska forskare för forskning hemma eller i utlandet samt för inbjudan av utländska gästforskare samt bidrag för att kvarhålla forskare inom landet. Sista ansökningsdag är 31 mars 2001. Info: Sascha Edblad, Monica Rosengren eller Sophia Westlund, 08-673 95 00, stipendier@kva.se. Web-info: http://www.kva.se/sve/pg/stipendier/var/matteans.asp.
13. Stiftelsen för internationalisering av högre utbildning och forskning (STINT) utlyser bidrag för kortare utlandsvistelser för lärare eller forskare vid svenskt universitet, högskola eller forskningsinstitut, dock ej doktorander. Ansökan kan inlämnas fortlöpande under året, dock senast 8 veckor före den dag då utlandsvistelsen avses påbörjas. Web-info: http://www.stint.se/KPutlys.html.
14. Anslag ställs, från Knut och Alice Wallenbergs Stiftelse, till rektors för KTH förfogande för att "i första hand användas till bidrag för sådana resor, som bäst befordrar ett personligt vetenskapligt utbyte till gagn för svensk forskning. Bidrag skall främst beviljas till yngre forskare." Ansökan om resebidrag skall ställas till rektors kansli. Bidrag kan sökas när som helst under året. Info: se punkt 5 ovan.
15. Nordisk Forskerutdanningsakademi (NorFA) finansierar nordiskt samarbete inom forskning och forskarutbildning genom dels personliga stipendier (mobilitetsstipendier och för deltagande i nationella forskarutbildningskurser), dels anslag till institutioner (forskarutbildningskurser, nordiska nätverk, gästprofessurer och workshops). Info: http://www.norfa.no.
16. Svenska Institutet (SI) utlyser kontinuerligt stipendier och bidrag för studier och forskning utomlands: stipendier för Europastudier, internationella forskarstipendier, Östersjöstipendier, Visbyprogrammet, m.m. Aktuell information om SI:s samtliga stipendiemöjligheter och ansökningshandlingar finns på SI:s hemsida: http://www.si.se.
17. Stiftelsen för internationalisering av högre utbildning och forskning (STINT) utlyser medel för att främja samarbete med universitet och högskolor i Republiken Korea (Sydkorea), Taiwan, Hongkong, Indonesien och Egypten. Ansökningar skall inlämnas minst 6 – 8 veckor före verksamhetsstarten, och medlen kan sökas löpande under året. Info: STINT, Skeppargatan 8, 114 52 Stockholm, 08-662 76 90. Web-info: www.stint.se.
18. Wenner-Gren Stiftelserna utlyser gästföreläsaranslag, avsedda att möjliggöra för svenska forskare eller institutioner att inbjuda utländska gästföreläsare. Anslag sökes av den inbjudande forskaren eller institutionen. Ansökan kan inlämnas när som helst under året. Web-info: http://www.swgc.org/.

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19. NUTEK stipends for stay in research institutions (not universities) in Japan. Short or long periods. For persons with or almost with doctoral degree. You can apply at any time. Info: Kurt Borgne, 08-681 92 65, kurt.borgne@nutek.se. Web-info: http://www.nutek.se/teknik2/intfou/bilateralt/stipendie.html.

Jobs, to apply for

20. Naturvetenskapliga forskningsrådet (NFR) utlyser en forskartjänst inom stokastiska processer, 15 december. Info: Natalie Lunin, 08-454 42 32. Web-info: se punkt 2 ovan.
21. Matematikcentrum vid Lunds tekniska högskola utlyser en doktorandtjänst i matematik med inriktning mot matematisk modellering, 20 december. Info: Gunnar Sparr, 046-222 85 28, Gunnar.Sparr@math.lth.se. Web-info: http://www2.lth.se/ledjobb/dokt/index_e.asp.
22. Matematikcentrum vid Lunds tekniska högskola utlyser en doktorandtjänst i matematik med inriktning mot industrimatematik, 20 december. Info: Gunnar Sparr, 046-222 85 28, Gunnar.Sparr@math.lth.se. Web-info: http://www2.lth.se/ledjobb/dokt/index_e.asp.
23. Matematikcentrum vid Lunds tekniska högskola utlyser en doktorandtjänst i numerisk analys, 20 december. Info: Achim Schroll, 046-222 05 94, Achim.Schroll@na.lu.se. Web-info: http://www2.lth.se/ledjobb/dokt/index_e.asp.

GRADUATE COURSE

Dževad Belkić:
The Principles and Methods of Quantum Scattering Theory / continued
(The Padé-Lanczos Algorithm)

Dževad Belkić is Guest Professor in "Mathematical Radiation Physics" at Karolinska Institutet, Stockholm. E-mail: belkic@radfys.ks.se.

The credit of the course is 5 p. It is given on one day per week (Monday) from January 22, 2001, to March 19, 2001.

The course is given at the Department of Physics, KTH, in room F 01, Lindstedtsvägen 24.

Literature: A textbook by Dževad Belkić, *The Principles and Methods of Quantum Scattering Theory,* Institute of Physics Publishing Ltd. (Bristol, England), to appear in March 2001[ISNP0750304960](http://bookmark.iop.org/bookpge.htm?ID=617983879-6410-59741210-D&book=493h).

Keywords: Collisions, spectroscopy, autocorrelation functions, signal processing.

Abstract: The Padé approximant (PA) to a power series is a quotient of two polynomials. The PA provides a meaningful result even when the original expansion diverges. It can significantly accelerate slowly converging sequences and series. As opposed to a (single) polynomal approximation, the PA can analytically continue general functions outside their definition domains. The PA is also an efficient solver of a generalized eigenvalue problem for the quantum-mechanical evolution/relaxation matrix **U** comprised of autocorrelation functions. This permits a unification of scattering and spectroscopy in the versatile setting of signal processing. The autocorrelation functions are generic and, therefore, can be computed theoretically and/or measured experimentally. Such a concept, born out as a computational tool, surpasses its initial purpose. *The autocorrelation functions represent a veritable alternative formulation of quantum mechanics.* This is not just because all the major observables, e.g., complete energy spectra, local density of states, quantal rate constants, etc., are expressible through the autocorrelation functions. It is also because these and other observables could be given completely in terms of some appropriate, relatively *small* informational parts that can be singled out and analysed separately from the unwanted/redundant remainder of the full data set of the autocorrelation functions. The needed dimensionality reduction of original large problems has previously been achieved within e.g. the Lanczos recursion,

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diagonalization methods or rational approximation techniques. Such methods are naturally ingrained in the Schrödinger picture of quantum mechanics or, equivalently, in the total time-independent Green's function of the studied system. This circumstance enables a unified treatment of spectroscopy and collision in the setting of signal processing. An example of such a versatile non-parametric and parametric estimator, the new Padé-Lanczos algorithm, is presently analysed for arbitrarily large signals without resorting to any kind of frequency windowing or decimation.

Introduction

A unified theoretical treatment of collisions and spectroscopy is outlined using the autocorrelation functions, $C(t) = (\Psi(0)|\Psi(t))$, with a natural link to signal processing. From the onset, this concept is rooted in basic quantum mechanics, since the state vector $\Psi(t)$ is the solution of the time-dependent Schrödinger equation, $\Omega\Psi(t) = i(\partial/\partial t)\Psi(t)$. In quantum mechanics of genuine bound states and a pure continuum, the dynamics of a considered physical system is described by a Hamiltonian H, which as a Hermitean operator, $H^\dagger = H$, coincides with Ω in the above Schrödinger equation for $\Psi(t)$. However, to include resonances via complex energy eigenvalues, as the most interesting part of scattering, we shall hereafter generalize the notion of a 'Hamiltonian' and extend it to encompass a non-Hermitean dynamic operator, Ω, in the same Schrödinger formalism. The deterministic postulate of quantum mechanics implies that if the wavepacket $\Psi(0)$ of the studied system is well prepared at the initial time, $t = 0$, the state $\Psi(t)$ will be known at any later instant t. Otherwise the state $\Psi(t)$ is the element of an abstract Hilbert vector space. Since $\Psi(t)$ is used to derive $C(t)$, it follows that this latter quantity also represents an abstract concept. This in itself immediately implies that autocorrelation functions, $C(t)$, are independent of the origin from which they are generated and, therefore, could be computed theoretically and/or measured experimentally as e.g. time signals, $c(t)$. As a matter of fact, the mathematical equivalence $C(t) = c(t)$ exists if a given time signal $c(t)$ is associated with a purely Lorentzian spectrum. In either case, the autocorrelation functions, $C(t)$, or the time signals, $c(t)$, physically represent the instantaneous *survival probability amplitude* of the corresponding time-dependent state $\Psi(t)$ of the examined system. This is important for at least two reasons: (1) experimental raw signals, $c(t)$, can be used directly, without necessarily relying upon the theory, to deduce *by computations* the basic observables for scattering and spectroscopy, such as cross sections, rate coefficients, etc. (2) measured time signals, $c(t)$, that are also identifiable as counts per channels, can be directly and dynamically intertwined with the theory on a deeper fundamental level.

The experimental resolution power of many instruments such as spectrometers is limited by a particular theory, which is the Fast Fourier Transform (FFT). This method should be complemented whenever necessary by other more powerful high-resolution parametric estimators. The latter processors are able to extract, directly from the measurements without any post-processing fits, the main spectral features, i.e., information about resonances. One of such nonlinear methods is the present Padé-Lanczos algorithm (PLA), which invests a relatively small computational effort to efficiently arrive at a high resolution and good signal-to-noise ratio. The PLA plays a twofold role as (i) a spectral estimator which gives only the shape of a spectrum and as (ii) a parametric estimator with the capacity of quantifying a spectrum by yielding positions, heights, widths and phases of each resonance or peak without rooting the characteristic polynomial or solving the generalized eigenvalue problem of the evolution matrix.

The PLA might be conceived as an interface to new experiments in scattering and spectroscopy with a possibility of reaching a substantially higher experimental resolving

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power than the one currently available. This has been demonstrated in ion-cyclotron resonance (ICR) mass spectroscopy and nuclear magnetic resonance (NMR) [1]. Such an achievement could be exploited in the future by building new spectrometers that are based on PLA which also provides *en route* the conventional FFT spectra (see also Ref. 2).

1. Green's resolvent

Irrespective of whether one is concerned with spectroscopy or collisions, the whole physics of any given system is ingrained in one single quantity, the full Green's function $(\zeta|G|\xi)$ in a given representation $\{(\zeta|\,,\,|\xi)\}$. Here,

$$G(\omega) = \frac{1}{\omega - \Omega + i\eta}\,, \tag{1.1}$$

is a resolvent known as Green's operator. Further, $\Omega \in \mathcal{H}$ is a dynamical operator which governs the development of the studied physical system, and $\mathcal{H}$ is the underlying Hilbert space of operators and state vectors. In quantum mechanics, Ω is the standard Hamilton operator H, in classical physics it could be a Lagrangean or Liouvillian and the like. The operator Ω need not be Hermitean and, therefore, we shall consider $\Omega^\dagger \neq \Omega$ thoughout, so that generally the eigenvalues $\{\omega_k\}$ $(1 \leq k \leq K)$ are complex numbers. The total number K of frequencies $\{\omega_k\}$ could be a finite or an infinite integer which does not need to be fixed or even known in advance. Even the usual Hamiltonians are often converted to complex operators through the concept of the non-Hermitean optical-type absorbing potentials that could mimic absorption of the incoming particle flux by the target. For the same purpose, a simple device could be used which is based upon the so-called adiabatic theorem from scattering theory. This amounts to a modification consisting of including the damping factor $i\eta$ from $G(\omega)$ directly into the total interaction potential $V \longrightarrow V\mathrm{e}^{-i\eta}$ which is a part of Ω. Alternatively, one could use the well-known complex coordinate method to produce the non-Hermitean 'Hamiltonian' Ω. The crucial practical advantage of these circumstances that render the operator Ω complex is that its spectrum does not need to explicitly include continuum states. Such states could be approximately represented by the pseudo-continuum, which is a collection of pure discrete states at complex energies encompassing both bound states and resonances. The full widths at half maxima of all the frequency peaks, that are imbedded in continuum to represent localized positive energy wave packets, determine the inverse lifetimes of each of the resonances in the spectrum of Ω. The infinitesimal number $\eta > 0$ secures regularity of $G(\omega)$ for the ω's that belong to the set of the eigenfrequencies $\{\omega_k\}$ of Ω. Once the calculation has been completed, the limit $\eta \to 0^+$ or $\eta \to 0^-$ should be taken depending whether the outgoing or incoming boundary conditions are used. The superscripts $\pm$ indicate that η should tend to zero through positive/negative numbers, respectively. Non-Hermiticity of Ω implies that the scalar product in the Hilbert space $\mathcal{H}$ is defined as the symmetric inner product $(\zeta|\xi) = (\xi|\zeta)$. Here, no conjugation is placed onto either of the two state vectors or 'orbitals' $(\zeta|$ or $|\xi)$ that both belong to $\mathcal{H}$. For convenience, we shall set the Planck constant $\hbar$ equal to unity, which will allow us to interchangeably use the frequency (ω) and energy (E) as synonyms, $E = \hbar\omega = \omega$. A method which can provide an adequate spectral representation of the total Green's resolvent $G(\omega)$ would represent the key input to a valid theory for scattering $(E > 0)$ *and* spectroscopy $(E < 0)$.

If $G(\omega)$ is available, then all the observables for a collisional and a spectroscopic phenomenon can be obtained from the general Green's function, $G_{\alpha\beta}(\omega) = (\Phi_{0\beta}|G(\omega)|\Phi_{0\alpha})$. The diagonal elements are obtained for $\Phi_{0\alpha} = \Phi_{0\beta} \equiv \Phi_0$ as:

$$G_{00}(\omega) = (\Phi_0|G(\omega)|\Phi_0), \tag{1.2}$$

where Φ_0 is an initial or a reference state. For example, the local density of states $n_{00}(\omega)$

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can be computed from the residues of $G_{00}(\omega)$ at its singularities,

$$n_{00}(\omega) = -\frac{1}{\pi} \lim_{\eta \to 0^+} \mathrm{Im}\{G_{00}(\omega)\}. \tag{1.3}$$

An arbitrary physical system is presently subjected to an analysis by the general stationary and time-dependent methods of quantum mechanics. In the former type of methods, the complete set of scattering states $\{\Psi_k\}$ of the Schrödinger operator $\omega - \Omega$ will be available by solving the stationary eigenvalue problem,

$$\Omega|\Psi_k) = \omega_k|\Psi_k) \quad ; \quad 1 \leq k \leq K. \tag{1.4}$$

As is well-known, the main postulate of quantum mechanics is that the whole information of a given physical system is contained in the wave function Ψ_k. This is coherent with Eq. (1.4) since Ω is assumed to carry the entire information of the investigated object. Such a statement of completeness of information is expressed through the closure relation, $\sum_{k=1}^{K} |\Psi_k)(\Psi_k| = \widehat{1}$, where K need not be finite, as we mentioned previously. In principle, the sum over k should include integration of the continuum part of the spectrum of Ω. This can be omitted as the non-Hermitean dynamic operator Ω includes all the resonances. Inserting this latter representation of the unity operator $\widehat{1}$ into $G(\omega) = G(\omega)\widehat{1}$ immediately leads to the following spectral representation of the Green's operator:

$$G(\omega) = \sum_{k=1}^{K} \frac{P_k}{\omega - \omega_k + i\eta} \quad , \quad P_k = |\Psi_k)(\Psi_k|. \tag{1.5}$$

where P_k is the projection operator. Obviously the Green's operator (1.5) can provide information of the studied physical system at any frequency ω and not just ω_k that belong to Ψ_k as opposed to the Schrödinger equation (1.4). Assume that we are given the eigensolutions $\{\omega_k, \Psi_k\}$, but *not* the 'pseudo-Hamiltonian' Ω itself. Then Ω could be retrieved from its implicit definition,

$$\Omega = \sum_{k=1}^{K} \omega_k P_k \quad , \quad f(\Omega) = \sum_{k=1}^{K} f(\omega_k) P_k, \tag{1.6}$$

for any scalar and/or operator function f. In a particular case with $f = 1/(\omega - \Omega + i\eta) = G(\omega)$, the result (1.4) follows again from Eq. (1.6). According to the Cauchy theorem, the operator $G(\omega)$ is fully determined by the complete set $\{\omega_k, P_k\}$ of its singularities ω_k (poles, branch points, cuts) and the operator residues P_k.

2. Padé-Lanczos algorithm (PLA)

The 'solution' (1.5) to the scattering problem is purely of a formal nature, since the input Ψ_k to P_k is the unknown result of the full stationary eigenvalue problem (1.4), which is just as difficult as the method of the Green's operator. This is only apparent since, in fact, the Green's function has many marvelous features that can reveal all the virtues of the studied physical system without ever knowing $\{\Psi_k\}$. One of the methods which avoids the need for $\{\Psi_k\}$ is a broad concept of the rational functions, the most prominent examples of which are the continued fraction (CF) or the closely related Padé approximant (PA). These methods can obtain the residues and poles of the Green's function, i.e., the entire information needed, without explicit construction of any of the eigenvectors. For example, the CF representation of the diagonal Green's function is $G_{00}(\omega) = \mathcal{G}_0(\omega)$, where $\mathcal{G}_n(\omega) = 1/[\omega - i\eta - a_n - b_{n+1}^2 \mathcal{G}_{n+1}(\omega)]$, which can also be written in the following explicitly expanded form:

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$$G_{00}(\omega) = \cfrac{1}{\omega - i\eta - a_0 - \cfrac{b_1^2}{\omega - i\eta - a_1 - \cfrac{b_2^2}{\omega - i\eta - a_2 - \cdots - \cfrac{b_{M-1}^2}{\omega - i\eta - a_M \cdots}}}}. \tag{1.7}$$

Here, a_n and b_n are precisely the same coupling parameters as in the Lanczos algorithm of wavepacket propagation with the underlying tridiagonalization of the 'Hamiltonian' matrix $\mathbf{\Omega}$. The tridiagonal matrix $\mathbf{J}_{\mathbf{\Omega}_K} = \mathrm{trid}_K[b, a, b]$, which originates from $\mathbf{\Omega}$, is a Jacobi $K \times K$ matrix, which is zero everywhere except on the diagonal and the two paradiagonals with the elements immediately to either side of the diagonal, $(\phi_n|\Omega\phi_n) = b_n$, $(\phi_{n-1}|\Omega\phi_n) = b_n$ and $(\phi_m|\Omega\phi_n) = 0$ for $|m-n| > 1$ with $(\phi_m|\phi_m)$ for any m. No matrix inversion is encountered in the CF. Moreover, all that is required to construct the Green's spectrum in the Eq. (1.7) is the set of the coefficients $\{a_n, b_n\}$ that can be computed recursively,

$$b_{n+1}|\phi_{n+1}) = \{\Omega - i\eta - a_n\}|\phi_n) - b_n|\phi_{n-1}) \tag{1.8}$$

with the initialization $|\phi_0) = |\Phi_0)$. This Lanczos algorithm is such that $|\phi_{n-1})$ is automatically normalized to unity and orthogonalized to $|\phi_n)$ and $|\phi_{n-1})$. However, by construction of the chain, it readily follows that $|\phi_{n+1})$ is also orthogonal to all the remaining previous elements $|\phi_{n-2}), \ldots, |\phi_0)$. This Lanczos orthogonalization is a low-storage method as opposed to the corresponding Gram-Schmidt (GS) orthogonalization which uses all states at each stage of the computation. Physically, the state $|\phi_n)$ is essentially the nth environment of $|\phi_0)$. But the coupling of $|\phi_n)$ with its surroundings is only significant with the two nearest neighbours or 'orbitals' $|\phi_{n+1})$ and $|\phi_{n-1})$. This means that the $(n+1)th$ iteration in Eq. (1.8) needs to store only two preceeding states $|\phi_{n-1})$ and $|\phi_n)$ since all other vectors can safely be overwritten. This extreme storage economy is the key to the success of the scheme (1.8) relative to the GS orthogonalization which requires a copy of the surrounding orbitals for each new state vector generated. Hence, the recursion (1.8) is one of the ways to create a *local* representation of the 'Hamiltonian' Ω which can be either a Hermitean or a complex symmetric operator.

The quest for this locality is natural in view of the fact that in practice one never needs the whole of the Green's resolvent, $G(\omega)$, but rather only a preassigned matrix element. An important example of such local information needed is $G_{00}(\omega)$ encountered in the local density of states, $n_{00}(\omega)$, which represents the intensity of each eigenvector. Physically, $n_{00}(\omega)$ describes the effect of the rest of the system onto its one selected part. Therefore, it is plausible that the examined local orbital itself should play the major role and that the successively more distant neighbours are expected to exhibit lesser effects. The Lanczos algorithm of nearest neighbours achieves this hierarchy of environments whose relative influence to the local density of states is explicitly weighted and displayed. This algorithm, in fact, describes the evolution of the system from a given initial state $|\phi_0)$. Each element of the set $\{|\phi_n)\}$ has the symmetry of $|\phi_0)$ as a result of the repeated action of Ω onto the initial state. If the set $\{|\phi_n)\}$ is required to contain functions of different symmetry, it will be necessary to consider different initial orbitals. The chain (1.8) does not contain those orbitals $|\phi_n)$ that are uncoupled to $|\phi_0)$ indicating the zero survival probability, $(\phi_n|\phi_0) = 0$, of the state vector $|\phi_n)$. Note that any matrix can be conveniently transformed into a Jacobi matrix. It is then clear that the chain model is equivalent to expressing the matrix $\mathbf{\Omega}$ as the corresponding Jacobi matrix or tridiagonalization matrix, $\mathbf{J}_{\mathbf{\Omega}_K}$. An original problem under study might be of a high dimension N, i.e., of a large number of degrees of freedom that could be strongly coupled to each other leading to a serious storage problem. In such a case, the standard diagonalization of the associated dynamic matrix $\mathbf{\Omega}$ would require N^2

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registers. This constraint can be dramatically relaxed to the amount of stores of only $2N$ if $\mathbf{\Omega}$ possesses a local representation stored in a compact form subjected to Eq. (1.8). The self-created orthonormal functions $\{\phi_n\}$ form a basis set which coincides with the orthogonalized Krylov states, $\{\Omega^n|\phi_0)\}$ $(0 \leq n \leq M)$. Here, the Lancsoz algorithm of tridiagonalization is the key step for converting the fully filled large matrix $\mathbf{\Omega}$ into its corresponding sparse J-matrix, $\mathbf{J}_{\mathbf{\Omega}_K}$. A subsequent diagonalization of $\mathbf{J}_{\mathbf{\Omega}_K}$ via e.g. a complex version of the modified QL algorithm leads to the sought set of the eigenvalues $\{\omega_k\}$ and the corresponding residues $\{d_k\}$. Here, $d_k = (\Phi_0|\psi_k)$ and $|\psi_k) = \sum_{m=1}^{K} A_{mk}|\phi_m)$, where the expansion coefficients $\{A_{mk}\}$ are generated recursively during the construction of the Lanczos states, $\{|\phi_k)\}$. The matrices $\mathbf{\Omega}$ and $\mathbf{J}_{\mathbf{\Omega}_K}$ have the common set of the eigenvalues $\{\omega_k\}$.

Construction of the Lanczos states, $\{|\phi_n)\}$, at large times, t, needed to resolve closely spaced frequency resonances, is a computer extensive procedure due to a direct and successive action of the operator Ω on each state $|\phi_n)$ leading to matrix-vector multiplications. However, the CF or the related PA is a powerful convergence accelerator, yielding the frequency spectrum (1.7) with a reduced number of terms $\{a_n, b_n\}$, and without the need for an explicit generation of $C(t)$. The meaning of the nearest neighbour setting within the CF is that the coefficients $\{a_n, b_n\}$ become increasingly less significant for determination of the local density of states, $n_{00}(\omega)$, as one progresses further down the continued fraction in Eq. (1.7). A truncation of the above continued fraction for $G_{00}(\omega)$ after K iterations permits an algebraic simplification of Eq. (1.7) to a sum of the rational fractions $\sum_{k=1}^{K} d_k/(\omega - \omega_k - i\eta)$, where ω_k and d_k are the poles and residues of $G_{00}(\omega)$, respectively. This is precisely the partial fraction expansion of the PA, $P_K(\omega)/Q_K(\omega)$ in the case of the first-order poles, where $P_K(\omega)$ and $Q_K(\omega)$ are the polynomials of the order $K-1$ and K, respectively. Hence, the CF from Eq. (1.7) should also give the PA to G_{00}. In such a case the eigenvalues $\{\omega_k\}$ are the roots of the denominator polynomial, $Q_K(\omega_k) = 0$, whereas d_k are the residues of $P_K(\omega)/Q_K(\omega)$. To obtain a link between the Lanczos method and the PA, we use the fact that the eigenvalues of the $K \times K$ matrix $\mathbf{J}_{\mathbf{\Omega}_K}$ are identical to the solutions of the corresponding secular equation, $\det(\omega\mathbf{1} - \mathbf{J}_{\mathbf{\Omega}_K}) = 0$ or, equivalently, to the zeros of the Kth order characteristic polynomial, $Q_K(\omega) \equiv \det(\omega\mathbf{1} - \mathbf{J}_{\mathbf{\Omega}_K})$. Given the tridiagonal structure, $\mathbf{J}_{\mathbf{\Omega}_K} = \mathrm{trid}_K[b, a, b]$, it is immediately apparent that both $P_n(\omega)$, and $Q_n(\omega)$ satisfy the same three-term recursion relation,

$$b_{n+1}T_{n+1}(\omega) = (\omega - a_n)T_n(\omega) - b_nT_{n-1}(\omega) \quad ; \quad T_n = P_n, Q_n. \tag{1.9}$$

To this recursion, two sets of different initial conditions such as $P_0(\omega) = 0$, $P_1(\omega) = 1$ and $Q_{-1}(\omega) = 0$, $Q_0(\omega) = 1$ are imposed so that the generated functions P_n and Q_n are the polynomials of the order $n-1$ and n, respectively. In other words, selecting the appropriate initialization, the same Lanczos recursion with the same definition of the coefficients a_n, b_n, applies to $\{|\phi_n)\}$ and $\{P_n, Q_n\}$. This means that the Padé ansatz $P_K(\omega)$, $Q_K(\omega)$ can be generated in the course of producing the Lancsoz states $\{|\phi_n)\}$ in K iterations with no additional effort yielding directly the PA to $G_{00}(\omega)$ as the polynomial quotient,

$$b_1G_{00}(\omega) = \frac{P_K(\omega)}{Q_K(\omega)}\,. \tag{1.10}$$

Such a PA to G_{00} is a meromorphic function, since the only singularities of this diagonal Green's function are assumed to be its poles. The zeros of P_K and Q_K are the zeros and poles of G_{00}, respectively. There are K poles of G_{00} since Q_K is a polynomial of the Kth order. When all the zeros of Q_K are distinct, the partial fraction expansion of the r.h.s. of Eq. (1.10) is given by

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$$b_1 G_{00}(\omega) = \frac{P_K(\omega)}{Q_K(\omega)} = \sum_{k=1}^{K} \frac{d_k}{\omega - \omega_k - i\eta} \quad , \quad d_k = \frac{P_K(\omega_k)}{Q'_K(\omega_k)}\,, \tag{1.11}$$

where $Q'_K(\omega) = (d/d\omega)Q_K(\omega)$. In here the residue d_k is given by an explicit analytical expression. If $\mathbf{J}_{\mathbf{\Omega}_K}$ were a real symmetric tridiagonal matrix, all its eigenvalues $\{\omega_k\}$ would be real and distinct so that the resulting spectrum is nondegenerate. However, the complex symmetric matrix $\mathbf{J}_{\mathbf{\Omega}_K}$ may have a degenerate spectrum and this occurs when some of the zeros of Q_K are mutually equal. In this case e.g. the kth complex root ω_k could have the multiplicity L, so that the partial fraction expansion of P_K/Q_K becomes:

$$\frac{P_K(\omega)}{Q_K(\omega)} = \sum_{k=1}^{K} \sum_{\ell_k=0}^{L} \frac{d_{k,\ell_k}}{(\omega - \omega_k - i\eta)^{1+\ell_k}} \quad , \quad d_{k,\ell_k} = \frac{P_K(\omega_k)}{Q_K^{(1+\ell_k)}(\omega_k)}\,, \tag{1.12}$$

with $Q_K^{(\ell_k)}(\omega) = (d/d\omega)^{\ell_k} Q_K(\omega)$. The Green's function, $G_{00}(\omega)$, and a time-dependent auto-correlation function, $C(t)$ are related by the standard Fourier integral which can be calculated analytically with the result:

$$C(t) = \sum_{k=1}^{K} d_k \mathrm{e}^{-i\omega_k t} \tag{1.13}$$

for the nondegenerate case containing the distinct poles $\{\omega_k\}$ and

$$C(t) = \sum_{k=1}^{K} d_k(t) \mathrm{e}^{-i\omega_k t} \quad ; \quad d_k(t) = \sum_{\ell_k=0}^{L} d_{k,\ell_k} t^{\ell_k} \tag{1.14}$$

for a degenerate spectrum where the kth zero has multiplicity L. In this latter case, the non-stationary amplitudes $\{d_k(t)\}$ emerge in the form (1.14) of a polynomial of order L in the time variable, $t \geq 0$. Interestingly, a special case of the real-valued auto-correlation functions, $C(t)$, from Eq. (1.14), containing exponentials with $\omega_k = -i\lambda_k$ ($\lambda_k > 0$) appear in the analysis of words.

3. Auto-correlation functions

An equivalent formalism is provided by the time-dependent Schrödinger equation,

$$i\frac{\partial}{\partial t}\Phi(t) = \Omega\Phi(t). \tag{1.15}$$

In the Schrödinger picture of quantum mechanics, operators are stationary and wave functions are time-dependent. For a stationary ansatz Ω, Eq. (1.4) possesses a solution of the type $\Phi(t) = U(t)\Phi_0$, where $\Phi_0 \equiv \Phi(0)$ is the initial state of the system at the time $t = 0$ and $U(t)$ is the evolution operator,

$$U(t) = \mathrm{e}^{-i\Omega t}. \tag{1.16}$$

In other words, if Ω and Φ_0 are known, then the determinism of quantum mechanics explicitly prescribes the exact knowledge of the state $\Phi(t)$ of the system at any later instant $t > 0$. As it stands, U is a non-linear operator due to the appearance of Ω in the exponential. We can 'linearize' U by using (1.6) which for $f = \mathrm{e}^{-i\Omega t} = U(t)$ becomes:

$$U(t) = \sum_{k=1}^{K} \mathrm{e}^{-i\omega_k t} P_k. \tag{1.17}$$

The state $\Phi(t)$ at the instant t is obtained by propagating the initial well-prepared wave

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packet Φ_0 from $t = 0$ to t via $U(t)$. Given Φ_0 at $t = 0$, there will be a non-zero probability amplitude to find the system in the state $\Phi(t)$ at the later time $t > 0$, if the two wave-packets have a non-vanishing overlap. This overlap is found quantum-mechanically by projecting $\Phi(t)$ onto Φ_0 by means of the their scalar product:

$$C(t) = (\Phi_0|\Phi(t)) = (\Phi_0|U(t)\Phi_0). \tag{1.18}$$

The quantitity $C(t)$ is called the autocorrelation function, since it measures the degree of correlations between $\Phi(t = 0)$ and $\Phi(t \neq 0)$ under the influence of the operator Ω. It is the presence of the dynamical operator Ω which makes $\Phi(t)$ differ from Φ_0 as is obvious from $\Phi(t) = \exp(-i\Omega t)\Phi_0$. By switching the dynamics off, the system would be allowed to remain indefinitely in the initial state, so that $C(t) = (\Phi_0|\Phi_0) = 1$ for $\Omega = 0$ at any time t. For unequal initial and final states, one introduces the so-called cross-correlation function, $C_{\alpha\beta}(t) = (\Phi_{0\beta}|U(t)\Phi_{0\alpha})$. At large times t, the autocorrelation function $C(t)$ is unreliable due to instabilities that stem from severe oscillations of $(\Phi_0|\Phi(t))$ as t increases. This could cause a heavy corruption of $C(t)$'s with a computational 'noise' e.g. round-off, ill-conditioning, etc. It is often stated in the literature that (1.2) exhibits singularities (poles, cuts, etc.) because of the presence of the resolvent (1.5) in $G(\omega)$. Also a claim that $C(t)$ is free from such singularities has frequently been put forward. The latter is, however, untrue. The reason being that the severe oscillations of $C(t)$ for large t, in fact, act as disguised singularities entirely similar to those encountered more transparantly in $G(\omega)$. This is obvious from the fact that both correlation functions $C(t)$ and $G(\omega)$ are built from the same 'Hamiltonian' Ω, which is an infinitesimal generator of the evolution operator $U(t)$. Moreover, the limits $t \longrightarrow \pm\infty$ in $C(t)$ are strictly equivalent to $\eta \longrightarrow 0^{\mp}$ in $G(\omega)$ in accordance with the so-called Abel limit. As a matter of fact, if one does not encounter instabilities in $C(t)$ in producing a spectrum, this could only mean that the indispensable asymptotic region $t \longrightarrow \pm\infty$, has not been reached and, therefore, the obtained result should be considered inadequate.

The above two representations, the stationary and the time-dependent one, are interrelated by means of e.g. the one-sided Fourier integral:

$$\mathcal{F}(\omega) = \int_0^\infty dt \mathrm{e}^{i\omega t} C(t). \tag{1.19}$$

With the help of the Dirac δ-function, the inverse Fourier transform of $\mathcal{F}(\omega)$ in the ω-space exactly retrieves $C(t)$ according to:

$$C(t) = \frac{1}{2\pi} \int_0^\infty d\omega \mathrm{e}^{-i\omega t} \mathcal{F}(\omega). \tag{1.20}$$

Both Eqs. (1.2) and (1.13) contain the same operator Ω which is the source of the complete information about the system. This feature together with unitarity of the standard Fourier operator guarantees that the information is preserved when passing from the time domain (t) to the frequency (ω) region. The quantities t and ω represent a pair of conjugate variables. Inserting (1.17) into Eq. (1.18) yields the result:

$$C(t) = \sum_{k=1}^{K} d_k \mathrm{e}^{-i\omega_k t} \quad , \quad d_k = (\Phi_0|\Psi_k)^2. \tag{1.21}$$

The quantities $\{d_k\}$ are the complex amplitudes that represent the residues associated with eigenfrequencies $\{\omega_k\}$ at pole ω_k. These residues measure the extent of the projection of the state Φ_k onto Ψ_0. In other words, the amplitudes $\{d_k\}$ are the weights carrying information on the strength of the contributions of individual normal mode frequencies $\{\omega_k\}$ to the

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signal's total power. More specifically, the magnitudes $\{|d_k|\}$ are the intensities of the harmonics $\{\mathrm{e}^{-i\omega_k t}\}$, featuring as the principal components that constitute the signal $C(t)$. Moreover, $\phi_k = \mathrm{Arg}(d_k)$ is the phase of $C(t)$. Substituting $C(t)$ from (1.21) into Eq. (1.19) and carrying out the time integral exactly gives the complex spectrum, $\mathcal{F}(\omega) = -i\sum_{k=1}^{K} d_k/(\omega - \omega_k + i\eta) \equiv -iF(\omega)$, where:

$$F(\omega) = \sum_{k=1}^{K} \frac{d_k}{\omega - \omega_k}\,, \tag{1.22}$$

provided $\mathrm{Im}(\omega_k) < 0$. The magnitude, power, absorption and dispersion spectra are obtained from: $|F(\omega)|$, $|F(\omega)|^2$, $A(\omega) = \mathrm{Re}\{F(\omega)\}$ and $D(\omega) = \mathrm{Im}\{F(\omega)\}$, respectively. The most important for experiments are absorption spectra, $A(\omega)$, which should be positive definite. In principle, the damping factor $i\eta$ need not necessarily be kept in Eqs. (1.21) and (1.22) as ω_k itself is complex for a non-Hermitean Ω. The overall result (1.22) is then a Lorentzian spectrum. This is expected as Eq. (1.22) corresponds to the autocorrelation function $C(t)$ which is given by a linear combination of attenuated exponentials (1.21). The resonance parameters from Eq. (1.22) are the position, width and height of the kth peak given by: $\mathrm{Re}(\omega_k)$, $\mathrm{Im}(\omega_k)$, $|d_k|$, respectively. The autocorrelation function $C(t)$ from Eq. (1.18) is identified with an instantaneous transition amplitude for a passage of the system from $\Phi(t)$ to $\Phi(0)$. Then the survival probability amplitude for the state $\Phi(t)$ is obtained in the limit of $C(t)$ for large times $|t| \longrightarrow \infty$. This time limit is crucial for any collision problem in order to secure that the full scattering states are reduced to the appropriate free wave packets. In spectroscopy, the epoch (T) of time-dependent observables must be sufficiently long to facilitate decays of all transient states so that the physically relevant transitions could be unambiguously detected.

In practice, one equidistantly discretizes (digitizes) the continuous (analogue) time variable t as $t = t_n \equiv n\Delta t$ $(n = 0, 1, 2, \ldots, 2M + 1)$, where now the integer n counts the time. The quantity $\Delta t \equiv \tau$ is the time increment (the time lag) or sampling time which is also called the 'dwell' time. The Schrödinger state at the time $t = t_n = n\tau$ will be denoted as $\Phi_n \equiv \Phi(n\tau)$. Due to the exponential nature of the evolution operator (1.16), construction of its discrete counterpart $U(n\tau)$ at the time $t = n\tau$ is done simply through raising the ansatz $U(\tau) = \mathrm{e}^{-i\Omega\tau}$ to the nth power:

$$U(n\tau) = U^n(\tau) \quad \Rightarrow \quad \Phi_n = U^n(\tau)\Phi_0\,. \tag{1.23}$$

Using this property, the discrete version of the autocorrelation function, denoted by $C(n\tau) \equiv C_n$ is given by:

$$C_n = (\Phi_0|\Phi_n) = (\Phi_0|U^n(\tau)\Phi_0). \tag{1.24}$$

Similarly, Eq. (1.21) can also be discretized according to the expression:

$$C_n = \sum_{k=1}^{K} d_k u_k^n \quad , \quad u_k = \mathrm{e}^{-i\omega_k\tau}. \tag{1.25}$$

It follows from here that the resonance parameters $\{\omega_k, d_k\}$, that are necessary for building each digital autocorrelation function c_n as a power series expansion in terms of the attenuated exponentials u_k, can be obtained by diagonalizing the evolution operator $U(\tau)$:

$$U(\tau)|\Psi_k) = u_k|\Psi_k). \tag{1.26}$$

This eigenvalue problem follows from Eqs. (1.4) and $f(\Omega)|\Psi_k) = f(u_k)|\Psi_k)$ for any function f. For diagonalization, one does need the explicit knowledge of the operator $U(\tau)$ itself,

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but only its matrix elements $(\chi_m|U(\tau)\chi_n)$ on a suitably selected complete set $\{\chi_n\}$ of the expansion functions χ_n that form a basis. The first such basis which naturally comes to mind is the set $\{\Phi_n\}$ of the Schrödinger functions $\Phi_n = U^n(\tau)\Phi_0$ from Eq. (1.23). In general, the two different 'orbitals' Φ_n and Φ_m are not mutually orthogonal, so that their overlap is $S_{nm} = (\Phi_m|\Phi_n) \neq \delta_{nm}$, where δ_{nm} is the usual Kronecker δ-symbol. However, the normalization is assumed to hold true, i.e., $S_{nn} = 1$. Completeness of the basis $\{\Phi_n\}$ permits a development of the eigenfunction Ψ_k of Ω from Eq. (1.26) as follows:

$$|\Psi_k) = \sum_{n=0}^{M} B_{nk}|\Phi_n), \tag{1.27}$$

where the expansion coefficients are the elements of the column matrix $\mathbf{B}_k = \{B_{nk}\}$. Then we insert this state vector into Eq. (1.26), which is afterwards multipled by $(\Phi_m|$, to arrive at:

$$\sum_{n=0}^{M} U_{nm}B_{nk} = u_k \sum_{n=0}^{M} S_{nm}B_{nk}. \tag{1.28}$$

Here, $\mathbf{U} = \{U_{nm}\}$ and $\mathbf{S} = \{S_{nm}\}$ are the evolution and overlap matrices, with the elements:

$$U^p_{nm} = (\Phi_m|U^p(\tau)\Phi_n) \;\; ; \;\; U^0_{nm} \equiv S_{nm} = (\Phi_m|\Phi_n), \tag{1.29}$$

where p is any positive or negative integer including zero. The system of linear equations in (1.28) can be succinctly rewritten in its corresponding matrix representation as:

$$\mathbf{U}\mathbf{B}_k = u_k\mathbf{S}\mathbf{B}_k, \tag{1.30}$$

where the expansion column matrix $\mathbf{B}_k$ from (1.27) is now the eigenvector. The obtained Eq. (1.30) is not an ordinary, but rather a generalized eigenvalue problem involving the overlap matrix $\mathbf{S}$, due to the mentioned lack of orthogonality of the Schrödinger basis functions Φ_m and Φ_n for $n \neq m$. With the basis set $\{\Phi_n\}$, the matrix element U^p_{nm} takes a particularly simple form which is obtained at once by inserting (1.23) into Eq. (1.29) and employing the symmetry property of the scalar product:

$$U^p_{nm}(\tau) \equiv (\Phi_m|U^p(\tau)\Phi_n) = (\Phi_0|U^{m+p+n}(\tau)\Phi_0) = c_{n+m+p}, \tag{1.31}$$

Hence, the matrix element of the pth power of the evolution operator $U(\tau)$ taken over two general Schrödinger states Φ_n and Φ_m is reduced to one single value of the autocorrelation function, c_{n+m+p}. Obviously, this result also includes the overlap matrix $\mathbf{S}$ for $p = 0$ as a special case of $\mathbf{U}^p$:

$$S_{nm} = (\Phi_m|\Phi_n) = c_{n+m}. \tag{1.32}$$

In general, $c_{n+m} \neq \delta_{n,m}$, which is compatible with the mentioned non-orthogonality of Φ_n and Φ_m for $n \neq m$. Once the whole set $\{u_k, B_{nk}\}$ is obtained by solving the generalized eigenvalue problem Eq. (1.28), the eigenfrequencies are deduced from $\omega_k = -i\ln(u_k)$. The corresponding residues d_k are calculated by inserting the expansion (1.27) for Ψ_k into Eq. (1.21) and using Eq. (1.24) for c_n with the result:

$$d_k = \left(\sum_{n=0}^{M} c_n B_{nk} \right)^2 \tag{1.33}$$

It is important to realize that Eqs. (1.30) and (1.33) represent yet another alternative formulation or picture of quantum mechanics with the central role played by the autocorrelation

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function c_n. This is because the diagonalization (1.30) of the evolution matrix $\mathbf{U}$ in the Schrödinger basis set $\{\Phi_n\}$ is all that one needs to obtain the entire spectral information (eigenfrequencies, residues, eigenfunctions, etc.) about the studied physical system whose time evolution is governed by the dynamical operator $U(\tau)$. All other physically measurable quantities could be computed from the set $\{\omega_k, d_k\}$. Note that the same Schrödinger basis set $\{\Phi_n\}$ employed to solve Eq. (1.30) has also been extensively used in quantum chemistry under the name Krylov functions. For practical purposes of solving Eq. (1.30), it is assumed that the size M of the basis set $\{\Phi_n\}$ is relatively small, say $M \leq 200$, implying that the linear programming in Eq. (1.26) can be done without severe round-off errors by using, e.g., the singular value decomposition (SVD) and the like. For larger values of M, a dimensionality reduction of the original problem is required via e.g. frequency windowing or band-limited decimation [3 – 10] (for an alternative approach without windowing or decimation, see Ref. 2). The amplitudes d_k from Eqs. (1.11) and (1.12) necessitate the knowledge of the eigenvectors $\{B_{nk}\}$. However, we have shown [1] that an explicit formula for d_k as in Eqs. (1.11) and (1.12) can be obtained without the need to compute any of the elements of the set $\{B_{nk}\}$, and this will be demonstrated in the present course. In the same course we will show how the auto-correlation function $C(t)$ can be obtained without using the set $\{\omega_k, d_k\}$ as opposed to the current practice which relies upon Eqs. (1.13) and (1.14). This very recent result of ours [1] is extremely important in practical computations in quantum chemistry, quantum physics, etc. The PLA can be applied to both experimentally measured signals c_n and theoretically computed auto-correlation functions C_n. In either case the PLA is shown to be an eigenvalue solver which is capable of yielding the complete set of eigenenergies, eigenfunctions and residues for both non-degenerate and degenerate spectra. The PLA obtains the Padé numerator and denominator polynomials $\{P_K, Q_K\}$ without any additional effort, since this is accomplished during the tridiagonalization of the dynamic 'Hamiltonian' $\mathbf{\Omega}$ by using the same coupling parameters $\{a_n, b_n\}$ encountered in the Lanczos states $\{\phi_n\}$ that are orthonormalized Krylov states. As opposed to Eq. (1.30) with the generalized eigenvalue problem of the operator $\mathbf{\Omega}$, the PLA solves an ordinary eigenvalue problem with the J-matrix $\mathbf{J}_{\mathbf{\Omega}_K}$ which is derived from $\mathbf{\Omega}$ by tridiagonalization. The two latter matrices are of the same dimension, but it is only the former which is sparse so that the dimensionality reduction is not necessary in the case when $\mathbf{\Omega}$ is a large matrix. If the matrix $\mathbf{\Omega}$ is unknown, but the auto-correlation functions $\{C_n\}$ or the signal points $\{c_n\}$ are given, the PLA tridiagonalizes the evolution matrix $\mathbf{U} = \exp(-i\mathbf{\Omega}\tau)$. In such a case, we have shown [1] that all the coupling parameters $\{a_n, b_n\}$ are defined solely in terms of $\{C_n\}$ or $\{c_n\}$. The auto-correlation functions $\{C_n\}$ and the time signals $\{c_n\}$ are equivalent to each other for purely Lorentzian spectra.

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