Orthogonal Polynomials and Special Functions

SIAM Activity Group on Orthogonal Polynomials and Special Functions

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Published Quarterly | Summer 1994 | Volume 4, Number 4

Contents

Edition Typeset June 10, 1994

The News

For those of us who must compute technical solutions, a useful preprint by Daniel Lozier and Frank Olver has recently appeared. It is called *"Numerical Evaluation of Special Functions"* and we quote from the Abstract: "Higher transcendental functions continue to play varied and important roles in investigations by engineers, mathematicians, scientists and statisticians. The purpose of this paper is to assist in locating useful approximations and software for the numerical generation of these functions, and to offer some suggestions for future developments in this field." Their paper will apear in *Mathematics of Computation 1943-1993: A Half-Century of Computational Mathematics*, Proceedings of Symposia in Applied Mathematics, American Mathematical Society, edited by Walter Gautschi. The preprint is available upon request from D.W. Lozier, Applied and Computational Mathematics Division, National Institute of Standards and Technology, Gaithersburg, MD 20899. Please be sure to give a postal mailing address. Dan's e-mail is dlozier@nist.gov.

Lectures on Hermite and Laguerre Expansions is the title of a 1993 book by Sundaram Thangavelu, published by Princeton University Press. From the preface: "This work deals with three types of expansions: 1) Hermite functions, 2) special Hermite functions, 3) Laguerre functions. For each type there are two basic questions: a) is the series convergent or summable in the L^p norm or almost everywhere for any L^p function? b) is a multiplier transform bounded on L^p if the multiplier satisfies a standard Hörmander condition, and if so how many derivatives are required? The results described in this work give a coherent account of what might be called the concrete Littlewood-Paley theory for a class of (related) expansions."

Two software packages on formal power series have been developed, one for Mathematica and one for Maple. These packages, together with the papers describing them, are available from Waleed Al Salam's ftp site, in the directories pub/koepf/pseries (for Mathematica) and pub/koepf/fps (for Maple). To access this site, type ftp euler.math.ualberta.ca (see the Summer 1993 Issue of this Newsletter for details).

(continues on p. 2)

The News *(continued)*

The final schedule for our Minisyposium in San Diego is now set, with twelve speakers in all. It begins Thursday afternoon, July 28, with four speakers, and then continues throughout Friday featuring the remaining eight speakers.

The OP-SF Net continues, under Tom Koornwinder's direction. The Net provides a fast turnaround. To *receive* the transmissions, just send your name and e-mail address to poly-request@siam.org (nonmembers can also receive the transmissions, as with other nets). Your OP-SF Net *contributions* should be sent to poly@siam.org. Please tell your friends and colleagues about the OP-SF Net.

The following announcement is taken from the OP-SF Net: Recently a grant has been approved for a program in special functions, q-series and related topics, to be held during June 12-23, 1995 at the Fields Institute in Toronto, Canada. Organizers are David Masson, Mizan Rahman and Mourad Ismail. The advisory committee consists of George Andrews, Richard Askey, Charles Dunkl, Tom Koornwinder and Doron Zeilberger (together with the organizers). During the first week of the program several minicourses will be given. In the second week there will be lectures on recent results, each day being devoted to a different topic. Further information about the program, possibilities of participation, etc., will follow later.

We regret that SIAM did not enclose the memberlist with the previous Newsletter, and that they also left out a few ads. It is expected that the memberlist will be included with this current edition, however, and that the ads will appear where they should be. Your editor apologizes for these omissions. Please note that the Newsletter is written and prepared in San Francisco by the editor, then shipped to Philadelphia for reproduction and mailing. Sometimes the geographical separation causes problems but we hope the kinks have been ironed out by now.

Workshop in Namur

Walter Van Assche has sent this summary of a recent gathering in Belgium:

On the 20th of May, 1994, a workshop was held at the Facultés Universitaires Notre-Dame de la Paix, in Namur, Belgium. Called a "Workshop on orthogonal polynomials: linearization and connection coefficients", it was organized by André Ronveaux of the Département de Physique in Namur. There were 5 talks, each of one hour length, and the speakers and the titles were:

- André Ronveaux (Facultés Universitaires N.D.P., Namur): *Introduction, survey, and some results for classical continuous and discrete families*
- Eduardo Godoy (Universidad de Vigo, Spain): *Recurrence relations for connection coefficients and integrals: computational aspects with* MATHEMATICA
- Walter Van Assche (Katholieke Universiteit Leuven): *Banach algebras associated with positive linearization coefficients in perturbation analysis*
- Alphonse Magnus (Université Catholique de Louvain): *Difference relations for semi-classical SNUL polynomials*
- Erik Koelink (Katholieke Universiteit Leuven): *Nonnegative linearization coefficients for q-Legendre polynomials*

The problem of linearization is to expand the product of two orthogonal polynomials as a Fourier series in the orthogonal polynomials, i.e.,

$$p_i(x)\,p_j(x) = \sum_{k=|i-j|}^{i+j} L_{i,j,k}\,p_k(x),$$

where $L_{i,j,k}$ are the linearization coefficients. Connection coefficients indicate how to write an orthogonal polynomial p_n as a Fourier series in another family of orthogonal

polynomials q_k $(k \geq 0)$, i.e.,

$$p_n(x) = \sum_{k=0}^{n} C_{k,n}\, q_k(x),$$

where $C_{k,n}$ are the connection coefficients.

André Ronveaux gave a survey showing how the linearization problem is equivalent to the evaluation of integrals involving the product of three orthogonal polynomials, and how the connection problem is related to the Cholesky factorisation of a Gram matrix. He showed how one can compute the linearization and connection coefficients when there are differential relations between the orthogonal polynomials, i.e., for classical orthogonal polynomials (or for semi-classical orthogonal polynomials) for which

$$\sigma(x)\, p_n'(x) = \sum_{k=n-s-1}^{n+t-1} b_{k,n}\, p_k(x),$$

for some polynomial σ. When such a *structure relation* is available, then one can compute the linearization coefficients and the connection coefficients recursively, as was explained by Eduardo Godoy who implemented the algorithms in MATHEMATICA. Quite often the positivity of the linearization coefficients is important, as was explained by showing that, in this case, a Banach algebra of polynomials can be constructed with an appropriate norm. This Banach algebra can be used to describe some properties of orthogonal polynomials which are obtained by small perturbations of the recurrence coefficients of a system of orthogonal polynomials with non-negative linearization coefficients.

After a good lunch (in Belgium, a lunch is always good), Alphonse Magnus showed how the classical orthogonal polynomials in the Askey table (Askey and Wilson) and the orthogonal polynomials on quadratic lattices (Nikiforov, Uvarov, Suslov) can all be considered as SNUL polynomials, where SNUL is an acronym for *Special Non Uniform Lattice* polynomials. Semi-classical SNUL polynomials are defined through a special difference equation, generalizing the ordinary difference and the q-difference operator. Finally Erik Koelink showed that the linearization of orthogonal polynomials often has a (quantum) group-theoretic interpretation, and how this can be of help in showing that linearization coefficients for certain families of orthogonal polynomials are non-negative.

The workshop was attended by approximately 15 persons.

Special Issue SIAM J. Math. Analysis

The March issue of the SIAM Journal of Mathematical Analysis, which has been dedicated to Richard Askey and Frank Olver, was mailed out to subscribers. Due to its enormous size of over 570 pages, production fell behind schedule and it was mailed late. Non-subscribers in the USA, Canada, and Mexico can order a single issue at a cost of $65.00. If you live outside these countries, the cost is $75.00. To order, please contact:

SIAM Customer Service Department
3600 University City Science Center
Philadelphia, PA 19104-2688
Phone: (215) 382-9800 Fax: (215) 386-7999
service@siam.org

The entire contents of this special issue are listed below. The guest editors were George Andrews, George Gasper, Mourad Ismail and Paul Nevai.

Contents
SIAM Journal of Mathematical Analysis
Special Issue, Vol. 25, No. 2, March 1994
Dedicated to Richard Askey and Frank Olver

(continues on p. 4)

Special Issue *(continued)*

George Gasper and Walter Trebels, *On necessary multiplier conditions for Laguerre expansions II.*

Jeffrey S. Geronimo, *Scattering theory, orthogonal polynomials, and q-series.*

William M.Y. Goh and Jet Wimp, *On the asymptotics of Tricomi-Carlitz polynomials and their zero distribution (I).*

Dharma P. Gupta and David R. Masson, *Watson's basic analogue of Ramanujan's Entry 40 and its generalization.*

Robert A. Gustafson, *Some q-beta integrals on $SU(n)$ and $Sp(n)$ that generalize the Askey-Wilson and Nasrallah-Rahman integrals.*

P. Heywood and P.G. Rooney, *On the Struve transformation.*

Mourad E.H. Ismail, *Asymptotics of Pollaczek polynomials and their zeros.*

D.S. Jones, *Asymptotic remainders.*

William B. Jones, Olav Njåstad, and Haakon Waadeland, *Application of Szegö polynomials to frequency analysis.*

E.G. Kalnins, W. Miller, Jr., and S. Mukherjee, *Models of q-algebra representations: the group of plane motions.*

Jean Letessier, *Some results on co-recursive associated Laguerre and Jacobi polynomials.*

Lee Lorch and Peter Szego, *Bounds and montonicities for the zeros of derivatives of ultraspherical Bessel functions.*

Doron S. Lubinsky and Vilmos Totik, *Best weighted polynomial approximation via Jacobi expansions.*

Stephen C. Milne, *The C_l Rogers-Selberg identity.*

Jolanta K. Misiewicz and Donald St. P. Richards, *Positivity of integrals of Bessel functions.*

Robert O'Malley, Jr. and Leonid V. Kalachev, *Regularization of nonlinear differential-algebraic equations.*

R.B. Paris, *A generalization of Pearcey's integral.*

Mizan Rahman and Sergei K. Suslov, *The Pearson equation and the beta integrals.*

G.-C. Rota and B.D. Taylor, *The classical umbral calculus.*

R. Simion and D. Stanton, *Specializations of generalized Laguerre polynomials.*

Renato Spigler and Marco Vianello, *Discrete and continuous Liouville-Green-Olver approximations: a unified treatment via Volterra-Stieltjes integral equations.*

W.J. Thron, *Truncation error for limit periodic Schur algorithms.*

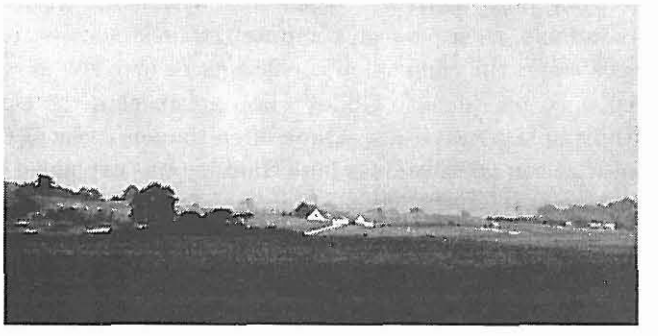
Galliano Valent, *Asymptotic analysis of some associated orthogonal polynomials connected with elliptic functions.*

R. Wong and J-M. Zhang, *On the relative extrema of the Jacobi polynomials $P_n^{(0,-1)}(x)$.*

Doron Zeilberger, *Towards a WZ evaluation of the Mehta integral.*

Due to conditions beyond the control of the guest editors, it was not possible to include in the same issue all papers that were accepted for publication. The two papers listed below will appear in future issues of the journal.

- Mizan Rahman and Sergei K. Suslov, *Barnes and Ramanujan-type integrals on the q-linear lattice.*
- Bo Gao, Donald J. Newman, and V.V. Popov, *Convex approximation by rational functions.*



Josef Meixner (1908–1994)

Professor Josef Meixner of the Technische Hochschule in Aachen, Germany, died on March 19, 1994. In April he would have reached his 86th birthday.

Meixner was well-known for his work on Meixner polynomials and Meixner-Pollaczek polynomials, and on Mathieu functions and spheriodal wave functions.

For details on his work, see especially his paper

> "Orthogonale Polynomsysteme mit einer besonderen Gestalt der erzeugenden Funktion",

which can be found in J. London Math. Soc. **9** (1934), pp. 6–13. And see especially also his books

1. *Mathieusche Funktionen und Sphäroidfunktionen* (with F.W. Schäfke)
2. *Mathieu Functions and Spheriodal Functions and Their Mathematical Foundations* (with F.W. Schäfke and Gerhard Wolf)

July Minisymposium in San Diego

At the SIAM Annual Meeting in San Diego, to be held July 25–29 this year, we will sponsor a Minisymposium. Charles Dunkl of the University of Virginia and Martin Muldoon of York University, Canada, are the organizers. The final schedule is now complete and is displayed below. It differs from the one given in the Preliminary Program mailed out by SIAM a few weeks ago.

The SIAM Minisymposium on
Asymptotics and Special Functions

July 28, Thursday Afternoon, 3:15–5:15 pm:

- Roderick Wong, City Polytechnic, Hong Kong. "Uniform asymptotic expansion of an oscillatory integral". mawong@cphkvx.cphk.hk
- Adri Olde Daalhuis, University of Maryland. "Hyperasymptotics". aod@olgao.umd.edu
- T. M. Dunster, San Diego State University. "New uniform asymptotic approximations for Jacobi polynomials". dunster@saturn.ucsd.edu
- Frank Stenger, University of Utah. "Asymptotic methods complemented by numerical methods". stenger@cs.utah.edu

July 29, Friday Morning, 10:00 am–12:00 noon:

- Richard Askey, University of Wisconsin. "Extensions of Hermite polynomials and other orthogonal polynomials". askey@math.wisc.edu
- Bruce Berndt, University of Illinois. "Some asymptotic formulas of Ramanujan". berndt@symcom.math.uiuc.edu
- Ronald Evans, University of California at San Diego. "Multidimensional q-beta integrals". revans@math.ucsd.edu
- George Gasper, Northwestern University. "Applications of sums and integrals of squares of special functions". george@math.nwu.edu

July 29, Friday Afternoon, 1:30–3:30 pm:

- Audrey Terras, University of California at San Diego. "Comparison of special functions for finite and continuous symmetric spaces". aterras@ucsd.edu
- Jeffrey S. Geronimo, Georgia Institute of Technology. "Asymptotics and spectral properties of orthogonal polynomials based on their recurrence coefficients". geronimo@math.gatech.edu
- Renato Spigler, University of Padua, Italy. "Discrete Liouville-Green approximations and orthogonal polynomial asymptotics". spigler@ipdudmsa.bitnet
- André Ronveaux, FUNDP, Namur, Belgium. "Heun's equations and the Schrödinger equation". aronveaux@cc.fundp.ac.be

For registration and other information please contact the SIAM office at

(215) 382-9800 (215) 386-7999 Fax
Toll Free: (800) 447-7426 (USA only)
meetings@siam.org

The meeting will be held at the Sheraton Harbor Island East Hotel, located right on San Diego Bay only minutes from the airport. For reservations call the hotel at (619) 291-2900 before July 5 and be sure to identify yourself as an attendee at the SIAM Annual Meeting in order to obtain the discount. And remember to get a confirmation number.

Future Minisymposia: Call for Topics

The Program Director of the Activity Group would like to receive your suggestions for future minisymposia. The program for San Diego is now already complete, so we are therefore interested in getting suggestions for the 1995 SIAM Annual Meeting (Louisville, October 16–19) and for the 1995 ICIAM Meeting (Hamburg, July 3–7). Normally a minisymposium would consist of around half a dozen 20–30 minute talks on a particular theme. Please send your suggestions to the Program Director

Martin E. Muldoon
York University
Department of Mathematics & Statistics
North York M3J 1P3 Ontario, CANADA

or just send an e-mail to muldoon@mathstat.yorku.ca. It would be nice to receive your suggestions before the 25th of July (so we can talk them over at the San Diego meeting in case you are not there). "Orthogonal Polynomials in Several Variables" has been mentioned as a possibility.

Meetings and Conferences

Only number **6** is new here, the others having appeared (with different numbers) in previous editions.

1. The 100th anniversary of T.J. Stieltjes' premature death will be commemorated in 1994-95. A number of activities have been planned for Delft (see **5** below), and also Toulouse.

In Toulouse there will be a colloquium in the Spring of 1995. The focus will be on continued fractions and moment problems, orthogonal polynomials, Laplace transforms, the Riemann hypothesis, and other topics. This will have a somewhat historical character. Contact:

Prof. J.-B. Hiriart-Urruty
Groupe d'Histoire des Mathématiques
de l'Université Paul Sabatier
118, Route de Narbonne
31062 Toulouse, France

2. The Joint Institute for Nuclear Research will hold an International Workshop on "Finite Dimensional Integrable Systems" in Dubna, Russia, July 18–21, 1994. The program includes invited talks as well as shorter contributions to be followed by discussions.

Among the topics to be discussed will be classical and quantum integrable systems (with n degrees of freedom), supersymmetry aspects of integrable systems, separation of variables and special functions, q-special functions, and q-groups. About 60 scientists from various centers are planning to attend.

Registration for participants will be US$ 250, and for companions it will be US$ 150. This covers meals and lodging during the Workshop, the transportation to Dubna from Moscow and return, the social program, and a volume of abstracts. Payments will be accepted by the Organizing Committee in Dubna during the registration. A program for companions is also planned.

A.N. Sissakian is chairman of the organizing committee; George S. Pogosyan (Dubna) and Pavel Winternitz (Montreal) are vice-chairmen. Please apply to George Pogosyan, with a copy to Pavel Winternitz.

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For your visas, accommodations, and transportation please contact Elena Pankova at the above address in Dubna. Fax: (7 095) 975 2381, Telex: 911621 dubna su, e-mail: pankova@cvxct0.jinr.dubna.su.

3. A Workshop on "Transform Methods and Special Functions" will be held in Sofia, Bulgaria, 12–17 August, 1994. The main subjects of the Workshop will be: Integral Transforms, Special Functions, Series Expansions, Fractional Calculus and Generalizations, Algebraical Analysis, Operational Calculus, Applications to Complex Analysis, Differential and Integral Equations.

Chairmen of the Organizing Committee are P. Rusev, I. Dimovski and S.L. Kalla. The venue will be the resort town of Bankya, 20 km from Sofia.

Full board for the entire period will be approximately US$ 150. This will include lodging and three meals. The registration fee for participants is US$ 100.

Since the rooms in Hotel Journalist should be booked long in advance, those who wish to participate are kindly asked to contact as soon as possible:

Prof. Virginia Kiryakova
Institute of Mathematics
Bulgarian Academy of Sciences
Sofia 1090, Bulgaria
Fax: (359 2) 752 078
virginia@bgearn.bitnet

4. Patrick Van Fleet of Sam Houston State University in Huntsville, Texas has indicated that a conference called "Special Functions and Their Applications" may be held during August 25–27, 1994. This is contingent upon funding and the following have tentatively agreed to speak.

George Andrews, Penn State University
Richard Askey, University of Wisconsin
Bille C. Carlson, Iowa State University
J. Dickey, University of Minnesota
Robert Gustafson, Texas A&M University
Edward Neuman, Southern Illinois University
V. Retakh, Harvard University
Roderick Wong, University of Manitoba

Graduate students are also encouraged to participate. Please contact

Patrick J. Van Fleet (mth_pvf@shsu.edu) or
Peter R. Massopust (mth_prm@shsu.edu)

Department of Mathematics
Sam Houston State University
Huntsville, TX 77341
Tel. (409) 294-1493

5. Also in commemoration of Stieltjes there will be a conference with the title "Orthogonality, Moment Problems, and Continued Fractions" to be held at the Delft University of Technology, October 31–November 4, 1994.

Each of four days will feature a different aspect of the work of Stieltjes, from continued fractions, rational approximation, moment problems, orthogonal polynomials, and asymptotics, to the properties of zeros and Gaussian quadrature. The format will consist of an invited lecture in the morning followed by short communications.

The invited lectures are

C. Berg, "Indeterminate moment problems and the theory of entire functions"

G. van Dijk, "Thomas Jan Stieltjes : mathematician by profession?"

J.B. Hiriart-Urruty, "Differentiability and non-differentiability in mathematical problems"

L. Lorentzen, "Continued fractions"

F. Marcellan, "Differential-difference operators and orthogonal polynomials in Sobolev spaces"

P. Nevai, "Generalized polynomials"

F. Peherstorfer, "Stieltjes polynomials and Gauss-Kronrod quadrature"

N.M. Temme, "Current problems in uniform asymptotic estimates of integrals"

W. Van Assche, "The impact of Stieltjes' work on orthogonal polynomials"

A second announcement, including a registration form, has already gone out. This can be obtained by sending a letter to

TJS94, Mekelweg 4, kr. H4.11
Department of Pure Mathematics
Delft University of Technology
P.O. Box 5031 2600 GA Delft
The Netherlands

or by sending an e-mail to tjs94@twi.tudelft.nl.

The Proceedings of the conference will be published as a special issue of the Journal of Computational and Applied Mathematics. Manuscripts must be submitted in triplicate during, or before, the conference.

Conference fees are Dfl. 600 for participants, including the program and book of abstracts, a copy of the proceedings, all lunches and dinners, coffee, tea, plus an excursion.

6. An International Symposium on "Methods and Applications of Analysis" will be held in Hong Kong, during December 16–19, 1994. The Program Organizers are

Robert M. Miura
Department of Mathematics
University of British Columbia
miura@neuron.math.ubc.ca

Roderick S.C. Wong
Department of Mathematics
City Polytechnic of Hong Kong
mawong@cphkvx.cphk.hk

Symposium topics will include asymptotics, integral equations, perturbation methods, special functions, and wave propagation. The symposium will not only provide a forum for an exchange of ideas among experts, but it will also disseminate information on recent advances made. There will be expository addresses, specialized talks, and poster sessions.

The Plenary Speakers are:

D.J. Benney, MIT
M.V. Berry, University of Bristol
C.K.R.J. Jones, Brown University
D.S. Jones, University of Dundee
M.D. Kruskal, Rutgers University
L. Lorch, York University
J.B. McLeod, University of Pittsburgh
M. Mimura, Tokyo University
F.W.J. Olver, University of Maryland
R.E. O'Malley, University of Washington

Call for Papers: Poster Session titles and abstracts must be received by July 30, 1994. The abstracts should be sent to one of the program organizers. They should be typewritten, double-spaced, and not exceed one page.

For additional information please contact Raymond Chan, Department of Mathematics, The Chinese University of Hong Kong. rchan@euler.math.cuhk.hk.

Problems

Thus far eight problems have been submitted while three have been solved (**#1, 4, 6**). A printout of all the problems and the solutions is available from the Editor.

2. Is it true that

$$x^2 t^x \, {}_2F_1(x+1,\, x+1;\, 2;\, 1-t)$$

is a convex function of x whenever $-\infty < x < \infty$ and $0 < t < 1$?

Submitted by George Gasper, August 19, 1992.
(g-gasper@nwu.edu)

3. The following Toeplitz matrix arises in several applications. Define for $i \neq j$

$$A_{ij}(\alpha) = \frac{\sin \alpha\pi(i-j)}{\pi(i-j)},$$

and set $A_{ii} = \alpha$. Conjecture: the matrix

$$M = (I - A)^{-1}$$

has positive entries. A proof is known for $0 < \alpha \leq 1/2$. Can one extend this to $0 < \alpha < 1$?

Submitted by Alberto Grünbaum, November 3, 1992.
(grunbaum@math.berkeley.edu)

5. The result of Problem #4 can be generalized to

$$\begin{aligned} S_m &= \sum_{n=0}^{\infty} \frac{(-1)^n (mn + 1/2)!}{\sqrt{\pi}\,(mn+1)!} \\ &= \frac{1}{m} \sum_{k=0}^{m-1} \frac{\sin\left(5(2k+1)\pi/(4m) + \pi/4\right)}{[2\sin\left((2k+1)\pi/(2m)\right)]^{1/2}} \end{aligned}$$

valid for integral $m \geq 2$.

Submitted by J. Boersma and P.J. de Doelder, July 12, 1993.
(wstanal@win.tue.nl)

7. The incomplete Airy integral given by [1]

$$I_0(\sigma, \gamma; k) = \int_{\gamma}^{\infty} e^{jk(\sigma z + z^3/3)}\, dz \qquad (1)$$

serves as a canonical integral for some sparsely explored diffraction phenomena involving the evaluation of high frequency EM fields [2] near terminated caustics and composite shadow boundaries. In equation (1), k is the wavenumber of the propagation medium and is assumed to be the large parameter. Both the parameters σ and γ are real.

The desired task is to derive a complete asymptotic expansion for I_0 in inverse powers of $k \to \infty$ for the case when the saddle points of the integrand satisfying

$$z^2 + \sigma = 0 \qquad (2)$$

$$z_{1,2} = \pm(-\sigma)^{1/2} \qquad (3)$$

are real and widely separated ($\sigma \ll -1$). The asymptotic expansion should be of the form

$$I_0(\sigma, \gamma; k) \sim \sum_{n=0}^{\infty} k^{-n} f(\sigma, \gamma, n) \qquad (4)$$

in which $f(\sigma, \gamma, n)$ is expressed in terms of known and easily computed functions. The asymptotic expansion in (4) should also hold uniformly as the endpoint γ approaches, or coincides with, one of the saddle points.

Submitted by E.D. Constantinides and R.J. Marhefka, August 11, 1993.
(evagoras@tiger.eng.ohio-state.edu)
(rjm@tiger.eng.ohio-state.edu)

8. Can the real and imaginary parts of a hypergeometric series of type ${}_pF_q$ with one complex parameter (either in the numerator or the denominator) be expressed by means of multiple hypergeometric series?

Submitted by Ernst D. Krupnikov, July 25, 1993.
(ernst@net.neic.nsk.su)

[1] Electrical engineers use j for $\sqrt{-1}$, reserving $i = v/r$ for current.

[2] See their brief article on electromagnetic (EM) diffraction in the Fall, 1993 issue of the Newsletter.

A Problem From Quantum Theory

by PAUL C. ABBOTT

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University of Western Australia
Nedlands, WA 6009 AUSTRALIA

paul@earwax.pd.uwa.edu.au

1. Introduction

In this note we sketch out the computation of the third order perturbation energy for the hydrogen molecular ion, arriving at a problem concerning the complementary exponential integral. See equations (2) and (3) towards the end of the note. Advice is sought on how to approach this problem.

We begin with the basic physics. The hydrogen atom perturbed by a point charge, or equivalently the hydrogen molecular ion in the fixed nucleus (Born-Oppenheimer) approximation, has been studied since the early days of quantum mechanics [1]. Consider the system of a hydrogen atom whose nucleus is located at the origin, perturbed by a point charge q at $(0,0,R)$. The unperturbed Hamiltonian is $H_0 = -\frac{1}{2}\Delta - \frac{1}{r}$. The Schrödinger equation for the unperturbed hydrogen atom, $(H_0 - E^{(0)})\Psi_0 = 0$, has the normalised ground state solution

$$\Psi_0 = \frac{1}{\sqrt{\pi}}\, e^{-r}, \quad E(0) = -\frac{1}{2}, \quad \langle \Psi_0 \mid \Psi_0 \rangle = 1.$$

When the interaction with the point charge is included, the Schrödinger equation becomes $(H - E)\Psi = 0$ where

$$H = H_0 + qV, \quad V = \frac{1}{R} - \frac{1}{X}, \quad X = (r^2 + R^2 - 2rR\cos\theta)^{1/2}.$$

2. Perturbation theory

Rayleigh-Schrödinger perturbation theory

$$\Psi = \sum_{n=0}^{\infty} q^n \Psi_n, \quad E = \sum_{n=0}^{\infty} q^n E^{(n)},$$

yields the system of equations

$$\begin{aligned}
(H_0 - E^{(0)})\Psi_1 &= (E^{(1)} - V)\Psi_0 \\
(H_0 - E^{(0)})\Psi_2 &= (E^{(1)} - V)\Psi_1 + E^{(2)}\Psi_0, \\
&\vdots \\
(H_0 - E^{(0)})\Psi_n &= (E^{(1)} - V)\Psi_{n-1} + \sum_{k=2}^{n} E^{(k)}\Psi_{n-k}.
\end{aligned}$$

Using the Hermiticity of the zeroth-order Hamiltonian and the orthonormality of Ψ_0 one obtains

$$\begin{aligned}
E^{(1)} &= \langle \Psi_0 | \, V \, | \Psi_0 \rangle \\
E^{(2)} &= \langle \Psi_0 | \, V \, | \Psi_1 \rangle - E^{(1)} \langle \Psi_0 \mid \Psi_1 \rangle \\
E^{(3)} &= \langle \Psi_1 | \, V \, | \Psi_1 \rangle - E^{(1)} \langle \Psi_1 \mid \Psi_1 \rangle - 2E^{(2)} \langle \Psi_0 \mid \Psi_1 \rangle .
\end{aligned}$$

Knowledge of the wavefunction up to Ψ_n allows the calculation of the perturbation energy up to $E^{(2n+1)}$. The first-order perturbation energy is easily evaluated:

$$E^{(1)} = e^{-2R}\left(1 + \frac{1}{R}\right).$$

The second order energy, which involves exponential integrals, can be found in [1].

3. First-order perturbation wavefunction

Substituting the *ansatz* $\Psi_1 = F\Psi_0$ into the first-order equation yields

$$\left(-\frac{1}{2}\Delta + \frac{\boldsymbol{r}\cdot\nabla}{r}\right) F = E^{(1)} - V. \tag{1}$$

In confocal elliptic coordinates:

$$\xi = \frac{r+X}{R}, \quad \eta = \frac{r-X}{R},$$

the potential reads

$$V = \frac{1}{R} - \frac{2}{R(\xi - \eta)},$$

and the volume element is

$$dV = r^2 \sin\theta \, dr \, d\theta \, d\phi = \frac{R^3}{8}(\xi^2 - \eta^2)\, d\xi \, d\eta \, d\phi,$$

in which $\xi \in [1, \infty)$, $\eta \in [-1, 1]$, and $\phi \in [0, 2\pi]$.

Denote the solution to (1) by $F_R(\xi, \eta)$. The linear partial differential equation for $F_R(\xi, \eta)$

$$\begin{aligned}
&\left[\frac{\partial}{d\xi}(\xi^2 - 1)\frac{\partial}{d\xi} + \frac{\partial}{d\eta}(1 - \eta^2)\frac{\partial}{d\eta}\right] F_R(\xi, \eta) \\
&\qquad -R\left[(\xi^2 - 1)\frac{\partial}{d\xi} + (1 - \eta^2)\frac{\partial}{d\eta}\right] F_R(\xi, \eta) = \\
&\qquad\qquad = -\frac{1}{2}R^2\left(E^{(1)} - \frac{1}{R}\right)(\xi^2 - \eta^2) - R(\xi + \eta),
\end{aligned}$$

can be solved by separation of variables and the application of the finite physical boundary conditions at $\xi = 1$, $\eta = 1$. One finds

$$\begin{aligned}
F_R(\xi, \eta) = \frac{R}{2}&\left(E^{(1)} - \frac{1}{R}\right)(\xi + \eta) + \\
&+ \left(1 + E^{(1)} - \frac{1}{R}\right)\log(\xi + 1) + d(R) \\
&+ \left(1 + \frac{1}{R}\right)\sum_{n=1}^{\infty} \frac{R^n(\eta - 1)^n}{n\, n!} \\
&- E^{(1)} \sum_{n=1}^{\infty} \frac{R^n(\eta + 1)^n}{n\, n!}.
\end{aligned}$$

(continues on p. 10)

A Problem From Quantum Theory *(continued)*

The integration constant $d(R)$ corresponds to the arbitrary amount of the zeroth-order eigenfunction present in the first-order eigenfunction.

Using the complementary exponential integral $\mathrm{Ein}(x)$, as defined in [2] and [3],

$$\mathrm{Ein}(x) = \int_0^x \frac{1-e^{-t}}{t}\,dt = -\sum_{n=1}^{\infty} \frac{(-x)^n}{n\,n!},$$

the solution can be written

$$\begin{aligned} F_R(\xi,\eta) = \frac{R}{2}\left(E^{(1)} - \frac{1}{R}\right)(\xi+\eta) + \\ + \left(1 + E^{(1)} - \frac{1}{R}\right)\log(\xi+1) \\ + d(R) - \left(1+\frac{1}{R}\right)\mathrm{Ein}(-R(\eta-1)) \\ + E^{(1)}\,\mathrm{Ein}(-R(\eta+1)). \end{aligned}$$

4. Third-order energy integrals

Computing the third-order energy requires evaluating the matrix elements (integrals) of $F_R(\xi,\eta)^2$. This leads to a number of integrals, most of which are simple. Terms such as

$$\int_{-1}^{1} e^{-R\eta}\,\mathrm{Ein}(-S(\eta-1))\,d\eta,$$

reduce to

$$\frac{e^R}{R}\,\mathrm{Ein}(2S) - \frac{e^{-R}}{R}\left(\mathrm{Ein}(2S-2R) - \mathrm{Ein}(-2R)\right).$$

The only integrals preventing a closed-form expression for the third-order energy are

$$\int_{-1}^{1} e^{-R\eta}\,\mathrm{Ein}(-S(\eta-1))\,\mathrm{Ein}(-T(\eta+1))\,d\eta, \qquad (2)$$

and

$$\int_{-1}^{1} e^{-R\eta}\,\mathrm{Ein}(-S(\eta-1))^2\,d\eta. \qquad (3)$$

All remaining integrals can be expressed in terms of these two by differentiation of parameters.

Advice as to how to reduce these integrals would be appreciated.

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[1] P. D. ROBINSON, Proc. Phys. Soc. **71**, 1958, pp. 828-842.

[2] M. ABRAMOWITZ and I. A. STEGUN, *Handbook of Mathematical Functions*, 1972, Dover.

[3] F.W.J. OLVER, *Asymptotics and Special Functions*, 1974, Academic Press. (Received March 18, 1994)

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\columnsep 0.25in
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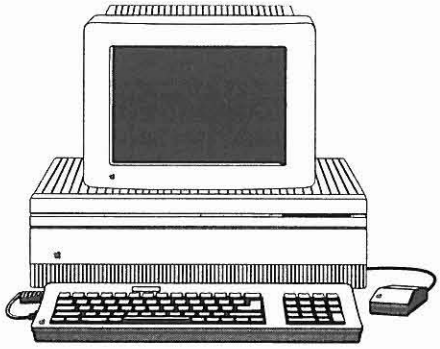

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