DEVELOPMENT OF q-CALCULUS FOR STUDIES OF MANY-PARTICLE QUANTUM SYSTEMS

THOMAS ERNST

1. CURRICULUM VITAE

Born in Uppsala 1960-08-17

1.1. **Early studies.** High school natural science 1979-06-08 in Malmö. Master of science in engineering physics 1985-10-21. In the last year of studies, we visitited DESY. In the period 1986-1995 I travelled a lot in Germany and visited other European countries. I also studied mathematics privately. In 1988 I was a student at the IBM school Böblingen 1988, the didactics was excellent. I was admitted as a graduate student of mathematics 1995. Doctor in mathematics at Uppsala November 14, 2002.

1.2. **Professional services.** 57 reviews in mathematics and physics for Zentralblatt Math.

Referee for the Bulletin of the Belgian Math. Society - Simon Stevin, J. of nonlinear mathematical phycics, Indian J. of math., Advan. Stud. Contemp. Math. (ASCM), Advances in Difference Equations.

My latest accepted paper was heavily influenced by reviews I had previously written.

Member of the grading committee, AbiTUMath Program at TUM during the conference on difference equations, Laufen, April 2007. The purpose was to collect high school and engineering students from Bavaria in a scientific atmosphere.

I taught q-calculus at two different occasions in Uppsala 2002 and 2006. Adviser (via e-mail) for Katheryne Merryl, university of Maine 2004.

Date: November 28, 2007.

1.3. **Conferences.**

1. 7th international Colloquium Quantum groups and integrable systems, Prague June 18-20, 1998 with talk.
2. European school in group theory, Leiden June 21 - July 4, 1998.
3. 4th international conference on lattice path combinatorics and applications, Vienna July 8-10, 1998.
4. Workshop on special functions and applications, Lund May 7, 1999 with talk.
5. Conference on q-Series with Applications to Combinatorics, Number Theory, and Physics, University of Illinois, October 26-28, 2000 with talk.
6. 10th international Colloquium Quantum groups and integrable systems Prague, June 21-23, 2001 with talk.
7. Conference on orthogonal functions and related topics, Röros, Norway, August 12 - 16, 2003, with talk.
8. Seventh international symposium on orthogonal polynomials, special functions and applications, Copenhagen August 18-22, 2003, with talk in parallel session.
9. International Conference on Difference Equations, Special Functions and Applications, Munich, July 25 - July 30, 2005, with talk.
10. Invited speaker Progress on Difference Equations, Bexbach, March 5-9, 2006.
11. Invited speaker Progress on Difference Equations, Salzburg, March 31 -April 5, 2007.
12. Orthogonal polynomials, Special Functions and Applications, Marseille, July 2007.
13. Invited speaker, conference in honor of Allan Peterson's 65th birthday, Novacella/Italy, July 28- August 2, 2007.

1.4. **Visit to.**

1. Mittag-Leffler institute May 1999 with talk and Jan.-June. 2005, with talks Feb. 22 and March 3.
2. Institute of theoretical physics at Munich, July 1999 with talk.
3. Penn state university October 23-24, 2000 with talk.
4. Wolfram research (Mathematica), Champaign, Illinois, October 29, 2000.
5. Institute of mathematics, Albert-Ludwigs-Universität Freiburg, June 13, 2001 with talk.
6. Visual Analysis AG (Mathematica), Munich, June 17, 2001.
7. Institute of mathematics at Vienna, June 19, 2001.
8. Institute of mathematical physics at Ulm, July 11-13, 2001.
9. Institute of mathematics i Stuttgart, July 2002.

(10) l'Institut d'electronique et d'informatique Gaspard-Monge Université de Marne-la-Vallée , Paris, with talk, January 17, 2003.
(11) RISC combinatorics group (Mathematica), Linz, Austria, January 20-21 with talk, May, 2003.

1.5. **Publications:**

(1) A method for q-calculus. *J. nonlinear mathematical physics* **10** No.4 (2003) 487–525.
(2) Some results for q-functions of many variables. *Rendiconti di Padova*, **112** (2004) 199–235.
(3) Generalized Cauchy-Vandermonde determinants, *Advan. Stud. Contemp. Math.* **11**, no. 1 (2005) 1-10.
(4) q-Generating functions for one and two variables. *Simon Stevin*, **12** no. 4, 2005, 589–605.
(5) q-Bernoulli and q-Euler Polynomials, An Umbral Approach. *International journal of difference equations* **1** no. 1 2006, 13-62.

1.6. **Self evaluation of research achievements.** I have been a kind of autodidact in q-calculus. Starting off in 1997, I tried to go through the whole literature on the subject, partly by using internet and our good library. After the first major publication, I turned to q-functions of many variables and Γ_q functions, partly assisted by Per Karlsson. In one of these papers I generalized formulas of my opponent Hari M. Srivastava, and showed the usefulness of the tilde operator. From 2003 I have studied q-Bernoulli and q-Euler Polynomials, and q-Stirling numbers. Although I consider myself an expert on this, this subject is not yet completed, and I know exactly how to continue. In the mean-time I have done some work on q-special functions and orthogonality to prepare for the continuation of the studies of q-functions of many variables. Through my many travels I have achieved a good knowledge of German and some knowledge of French, which makes it possible to study the literature in the field.

1.7. **Funding ID.** The only existing funding is an application of 1000 Euro from the Swedish research council for the ensuing conference in Marseille.

A grant should be used to preserve an existing team, which will work for another year.

2. THE RESEARCH PROJECT

2.1. **Introduction.** In this section we summarize the state-of-the-art and objectives of the project. In the second section we give a survey of special functions, including q-calculus. In the third section we summarize the mathematical methodology. In the fourth section we summarize the applications in physics. In the fifth section we describe the team and the role of each member.

My scientific work concerns q-calculus. q-calculus is one of the languages for algebraic combinatorics and started simultaneously with analytic number theory or theory of partitions about 250 years ago.

The investigator's programme is aimed at bringing the theory of q-calculus to a like degree of maturity to that enjoyed by hypergeometric series and elliptic functions, especially in view of current applications to quantum physics.

This leads to a new method and new notation for computations and classifications of q-special functions. With this method many formulas of q-calculus become very natural, and the q-analogues of many orthogonal polynomials and functions assume a very pleasant form reminding directly of their classical counterparts. Progress in q-calculus is heavily dependent on the use of a proper notation. It should thus be noted that q-calculus has wideranging applications in quantum theory, number theory, statistical mechanics and chemistry. A book about this subject is in preparation.

2.2. **What is special functions including q-calculus?** q-Calculus is a part of the AMS code 33, called special functions, which is intimately connected to differential equations, difference equations, Bernoulli numbers, and umbral calculus. The umbral calculus, with AMS code 05A40 and part of enumerative combinatorics, has different roots. The first goes back to Grünert, Gudermann, Kramp, and Schlömilch. The second one goes back to J. Herschel, Murphy, Boole, Heaviside, Horner, Blissard, Sylvester, Glaisher, and F. H.Jackson.

There is a connection to astronomy, spherical trigonometry, Stirling numbers, elliptic functions, which will be further illuminated by studies of the old Latin literature in the field. There are Russian and Italian contributions to the subject, the first one through Bernoulli numbers and the second through the author Toscano, which necessitate philological support to the project. The Latin team member can be found in the team list.

The q-hypergeometric series was developed by Heine 1846 as a generalization of the hypergeometric series. Heine proved beautiful transformation formulas for q-series by a purely formal calculation on continued fractions. In his work 1893-1895, Rogers inspired by Heine's book 'Handbuch der Kugelfunktionen', introduced a set of orthogonal polynomials which can be expressed in terms of q-hypergeometric series and which have the Gegenbauer polynomials as limits when $q \to 1$. In 1909 Ramanujan wrote to professor Hardy from India and told him about a number of identities which he could not prove. Some of them were just corollaries of the Rogers-Ramanujan identities. W.N.Bailey had been greatly influenced by Ramanujan as an undergraduate at Cambridge 1914. L.J. Slater attended Bailey's lectures on q-hypergeometric series in 1947-50 at Bedford College, London University and in 1966 published a book about generalized hypergeometric functions; among her pupils was H. Exton. Slater and Exton brought q-calculus into the computer age and Exton wrote the first book entirely devoted to q-series.

The theory of multiple hypergeometric functions developed by, among others, Hari M. Srivastava (British Columbia), Per Karlsson (Lyngby) and Exton is closely connected to this; Karlsson and Srivastava have written a monograph about this subject.

The so-called Heine q-umbral calculus reached its peak in the thesis by Smith 1911, supervised by Pringsheim. The Austrian school of q-analysis started in the sixties when Wolfgang Hahn (1911-1998) (graduate student of Schur in Berlin) moved to Graz in 1964 after visits to India 1959-1961 and America 1962. Because of Hahn's sojourn in India, and due to the fame of Ramanujan, q-calculus is today very popular in India.

There is also an equivalent operator theory based on the Gauss q-binomial coefficients developed by Johann Cigler (1937-) in Vienna, which I will come back to.

2.3. **Mathematical methodology.** The PI has introduced an umbral approach in the spirit of Rota for q-calculus, which should prove useful when proving new formulas in the huge subject special functions. The main ingredients are an infinite alphabet, the tilde operator (generalized to a root of unity), two types of dual q-additions, one is commutative, and the other one can be written as a finite product. The so-called q-complex numbers in n dimensions are a part of this alphabet; the q-holomorphic functions are the formal power series. The q-derivative will be extended to functions of q-complex numbers, and q-Cauchy-Riemann equations will be proved. My recent research has encompassed certain q-Bernoulli- and q-Euler polynomials, which has resulted in a q-Euler-MacLaurin expansion for formal power series. I have also treated q-Stirling numbers, which can be used to compute the speed of an algorithm.

In a previous paper from Rendiconti di Padova I have generalized some of Srivastava's formulas by using the Γ_q function; this is a project that will continue.

In the process of q-deformation of the hypergeometric function, a branching singularity $x = 1$ disappears and is replaced by an infinite number of poles and zeros. In order to find certain new q-formulas, some proofs use Jacobi theta functions. In my earliest papers, two formulas for generalized

Cauchy-Vandermonde determinants were proved. It seemed at first that this was research isolated from q-calculus. However it turned out that the previous work on q-Bernoulli- and q-Euler polynomials could be translated to matrix language. And suddenly the formulas about Pascal matrices could be q-deformed and q-analogues for special cases of Cauchy-Vandermonde determinants could be found. One example is a Cauchy-Vandermonde determinant with integer powers replaced by their q-analogues. The proof uses another form of q-Stirling numbers.

2.4. **Applications in physics.** We will now describe the reason why physics is so much involved in q-calculus. John von Neumann and Wigner introduced group representation theory to quantum mechanics. Based on his lectures on quantum mechanics in Göttingen 1926–27, David Hilbert formulated the mathematical description which is included in John von Neumann's collected work. q-deformed symmetries in physics are described by quantum groups and these are represented by q-special functions. In particular, to obtain the q-spherical harmonics, we only have to represent $SU_q(2)$.

The special mathematics which builds up q-calculus gives an alternative way of solutions to differential equations, so-called q-difference equations. It is therefore suited for physical applications, and many such applications have already been found in mechanics and theory of electricity. So far, q-analogues have been formulated for fundamental constituents in the solution of the Schrödinger equation, like Legendre polynomials, but further extensions are, to the best of our knowledge, missing. As such polynomials can be part of the treatment of many-electron-systems, this research can also encompass such atoms. The present project aims at more general formulations of q-analogues for interactions involved in many-electron systems treated on a particle basis and thus giving opportunities to account for electron correlation in atoms and molecules. We have a very big experimental material to compare with, and the methodology will be done in close connection to research groups in atomic- and molecular physics. Besides studies of electronic states, the methods will be tested for molecular vibrations and rotations. The experimental research within the present team involves both optical spectroscopy and photoelectron spectroscopy with vibrational resolution as well as multicoincidence experiments for studies of the electronic structure of atoms and molecules in different charge states and different states of fragmentation. The experiments are performed both at local laboratories and at synchrotron radiation laboratories. It may be noted that by the latter light sources, photon energies can be used that are sufficient for studies of the entire valence region including the inner valence.

For the latter, many-electron transitions are common and spectra are usually very complex due to a large number of states. These states are difficult to handle theoretically, and very time and effort consuming computer simulations have to be carried out generally today. Here, it would be of great interest to try new mathematical formalisms, and q-analysis gives such an opportunity. This q-theory can also be applied to quarks. The team around J. Wess has investigated the so-called q-Dirac equation.

2.5. **Team members.** We describe the research group and their responsibilities. The first four people won't require any payment from ERC.

(1) Dr. Martin Bohner Rolla, Missouri. Editor of two journals in difference equations. Responsible for advertising the project in the US.
(2) Prof. Leif Karlsson, physics dep. Uppsala univ. Responsible for atomic and molecular measurements. A very social person, who gives a lot of advice.
(3) Emma Previato, Boston University. Responsible for Theta functions, Latin and Italian texts, consulting.
(4) Per Karlsson, DTU Lyngby. Expert on hypergeometric functions of many variables, special functions, reviewer for Zentralblatt Math., book author. We meet about once a year in Copenhagen.
(5) Priv-Doz. Dr. Andreas Ruffing TU Munich. Expert on basic partial difference equations, difference operators in quantum mechanics. Conference organizer.

3. Research environment

3.1. **Transition to independence.** The project will enable the PI to travel to different conferences and thus consolidating his position as independent research leader in q-calculus.

3.2. **Resources in Sweden.** The hosting institution at Uppsala university has a good mathematical library consisting of old and new books, plus possiblity to order any book or article from Europe or the US. This library also offers online access to many math. journals. There is also the ancient university library (Carolina rediviva) in Uppsala, the Mittag-Leffler library in Djursholm, and the Stockholm mathematical library. At the mathematics department in Uppsala there are regular seminars in algebra, topology and analysis. There is an outstanding computer network for Linux machines hosted by two computer experts, Carl Edström and Christian Nygaard. The *Mathematica* program, often used by the PI is installed.

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