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ADVANCED METHODS FOR THE COMPUTATION OF PARTICLE
BEAM TRANSPORT AND THE COMPUTATION OF
ELECTROMAGNETIC FIELDS AND BEAM-CAVITY INTERACTIONS

Progress Report
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1 INTRODUCTION

The University of Maryland Dynamical Systems and Accelerator Theory Group has been carrying out long-term research work in the general area of Dynamical Systems with a particular emphasis on applications to Accelerator Physics. This work is broadly divided into two tasks: The Computation of Charged Particle Beam Transport and the Computation of Electromagnetic Fields and Beam-Cavity Interactions. Each of these tasks is described briefly below. Work is devoted both to the development of new methods and the application of these methods to problems of current interest in accelerator physics including the theoretical performance of present and proposed high energy machines.

In addition to its research effort, the Dynamical Systems and Accelerator Theory Group is actively engaged in the education of students and post-doctoral research associates. To this end, it presents a regular graduate seminar course in accelerator physics, directs graduate students in M.S. and Ph.D. thesis research, and guides and fosters the research of Post-doctoral Research Associates and Visiting Scientists.

Substantial progress in research has been made during the past year. There have also been important educational accomplishments. These achievements are summarized in the following report.

1.1 Task A: Charged Particle Beam Transport

A new method, employing Lie algebraic tools, has been developed for the computation of charged particle beam transport and accelerator design. It represents the action of each separate element of a beamline or accelerator, including nonlinear effects, by a certain operator. These operators can then be combined, following well-defined rules, to obtain a resultant transfer map that characterizes the entire system.

Lie algebraic methods may be used for particle tracking around or through a lattice and for analysis of linear and nonlinear lattice properties. When used for tracking, they are both exactly symplectic and extremely fast. Tracking can be performed element to element, lump to lump, or any mixture of the two. (A lump is a collection of elements combined together and treated using a single net transfer map.) The speed for element to element tracking is

comparable to that of other tracking methods. When collections of elements can be lumped together to form single transfer maps, tracking speeds can be orders of magnitude faster.

In addition to single particle tracking, Lie algebraic methods may also be used to determine how particle phase-space distribution functions evolve under transport through both linear and nonlinear elements. These methods are useful for the self-consistent treatment of space-charge effects and for the study of how moments and emittances evolve. They also provide a means for characterizing beams in terms of invariant eigen-emittances.

Lie algebraic methods also provide powerful means for carrying out analytic computations. Such computations include the calculation of first, second, and higher order chromaticities; first, second, and higher order dispersion; the dependence of tune on betatron amplitude; nonlinear lattice functions; nonlinear phase-space distortion; transfer map normal forms; nonlinear structure resonances; nonlinear beam-beam effects; and nonlinear invariants.

Finally, Lie algebraic methods can be used to give an explicit representation for the linear and nonlinear properties of the total transfer map of a system. This information can be used to evaluate or improve the optical quality of a single-pass system such as a beam transport line or linear collider. For example, it is possible to design high-order achromats, and aberration-corrected telescopes and final focus systems. For a circulating system such as a storage ring, explicit knowledge in this case of the one-turn transfer map can be used to predict the linear aperture of the system without the need for long-term tracking. It is hoped that eventually knowledge of this map can also be used to make predictions about the dynamic aperture of the system.

Presently the program MARYLIE 3.0 implements these methods through third order. More advanced and higher order versions of MARYLIE are under development.

Lie algebraic methods are also applicable to many other areas including the design of high resolution electron microscopes and microprobes; the design of low energy wide acceptance spectrometers; light optics; and many other problems in the field of dynamical systems. Work is also being carried out in some of these areas.

1.2 Task B: Computation of Electromagnetic Fields and Beam-Cavity Interactions

The next generation of linear colliders involves higher current beams of low emittance and short bunch length. The image currents produced by such beams generate wakefields which are capable of inducing instabilities in the beam. Accurate methods are needed to calculate these wakefields for iris loaded cavities and to analyze corrective measures intended to suppress these instabilities, such as BNS damping, autophasing, and detuning.

The next generation of high energy proton rings (LHC) enters a parameter region where synchrotron radiation becomes increasingly important. Insertions into the beam pipe are needed to remove the heat generated and to shield the beam pipe, usually operated at liquid helium temperatures, from the fields due to the circulating beam. The present plan is to insert a liner with holes into the beam pipe. Methods have been developed to calculate the wakefields induced by such a liner, as well as the penetration of the fields due to the circulating beam into the region between the liner and the beam pipe.

The penetration of electromagnetic fields through small holes in a thick wall enters into a variety of problems of current interest. These include the coupling of wave guides to cavities, the construction of an accurate equivalent circuit for an iris loaded cavity, the design of beam position monitors, and the generation of wakefields by holes in a liner within a beam pipe. Methods are needed to extend the calculation, first done by Bethe in 1944 for circular and elliptical holes in a zero thickness wall for long wavelengths, to the case of thick walls and shorter wavelengths.

High current ion linacs are known to develop beam halos. In order to avoid excessive activation of the linac it is essential to understand and control the origin of the halos. We are studying a possible model involving a resonant interaction between an oscillation mode of the beam core (such as a "breathing" mode) and the non-linear oscillation of individual particles.

2 Educational Accomplishments

One of the major goals of the Dynamical Systems and Accelerator Theory Group is the education of students, postdoctoral research associates, and visiting scientists. Listed below are present and past students associated with the program, and present and past postdoctoral research associates and visiting scientists.

2.1 Faculty

Alex J. Dragt, Professor of Physics

Robert L. Gluckstern, Professor of Physics

2.2 Visiting Professor

Dr. Iliya M. Kapchinsky was a Visiting Professor of Physics and Electrical Engineering from February 1, 1993 to April 30, 1993. During his visit he interacted with graduate students and many colleagues (both from Maryland and nearby Government Laboratories) who took advantage of his vast expertise in many aspects of accelerator theory. In addition, he presented about 10 lectures on the theory of linear accelerators. Unfortunately Dr. Kapchinsky died May 2, 1993, before he was able to return to Russia. In recognition of the widespread interest in his achievements and perspectives on these subjects, and as a service to the Accelerator Science Community, his lectures notes have been assembled and have been issued and broadly circulated as a Los Alamos Report.

2.3 Present Graduate Students

Dan Abell

Thesis work in progress on the computation and analytic properties of transfer maps, symplectification methods, and other topics in charged particle beam transport.

Wen-Hao Cheng

Now in his fourth year as a Graduate Research Assistant. He has completed

a study of an alternating phase focussing linac and a study of the frequency dependence of the polarizability of a hole in a thick plate. He is now working on the instability of a mismatched K-V beam.

Alexei Fedotov

First year Graduate Research Assistant. Working on the frequency dependence of the susceptibility of a hole in a thick plate.

Shicheng Jiang

Now in his third year as a Graduate Research Assistant. He has completed work on the longitudinal and transverse impedances of a thick iris, and is well on the way to completion of a corresponding calculation for periodic thick irises. He is also starting to work on the polarizability and susceptibility of a rectangular hole in a thick plate.

Marco Venturini

First year graduate student presently supported by Italian Government. Has worked in past at CERN on charged particle beam transport, and is expected to undertake thesis work in this general area.

2.4 Present Ph.D. Professional Staff

Sergey S. Kurennoy, Postdoctoral Research Associate.

Huanchun Ye, Postdoctoral Research Associate.

2.5 Past Graduate Students

David Douglas, Ph.D. 1982.

Thesis: Lie Algebraic Methods for Particle Accelerator Theory.

Employment: Previously employed by the Lawrence Berkeley Laboratory.

Presently employed by the Continuous Electron Beam Accelerator Facility.

Etienne Forest, Ph.D. 1984.

Thesis: Lie Algebraic Methods for Charged Particle Beams and Light Optics.

Employment: Lawrence Berkeley Laboratory.

Janko Milutinovic, Ph.D. 1984.

Thesis work done in Elementary Particle Theory while simultaneously receiving training in Accelerator Theory.

Employment: Accelerator Theory at Brookhaven National Laboratory.

Liam Healy, Ph.D. 1986.

Thesis: Lie Algebraic Methods for Treating Lattice Parameter Errors in Particle Accelerators.

Employment: Previously at CERN. Presently with Celestial Mechanics Group at the Naval Research Laboratory.

Robert Ryne, Ph.D. 1987.

Thesis: Lie Algebraic Treatment of Space Charge.

Employment: Previously employed by Lawrence Livermore National Laboratory. Presently employed by the Los Alamos National Laboratory.

Petra Schuett (1987-88).

Worked one year at Maryland on Lie algebraic methods and Poisson solvers while simultaneously completing her Ph.D. thesis work on Wake-Field Acceleration under Thomas Weiland at DESY.

Employment: Theoretische Elektrotechnik Group at the Darmstadt Technische Hochschule.

Govindan Rangarajan, Ph.D. 1990.

Thesis: Invariants for Symplectic Maps and Symplectic Completion of Symplectic Jets.

Employment: Previously at Lawrence Berkeley Laboratory. Now a member of the Mathematics Faculty, Indian Institute of Science, Bangalore, India.

Rui Li, Ph.D. 1990.

Thesis: Analytical and Numerical Investigation of the Longitudinal Coupling Impedance.

Employment: Continuous Electron Beam Accelerator Facility.

John Diamond, M.S. 1990.

Spent two years as a Graduate Research Assistant working on the penetration of electromagnetic fields through circular holes in a thick metallic wall. Also carried out symbolic manipulation program calculations for various complicated beamline elements such as combined-function quadrupoles and combined-function bends. In addition, responsible for general computational support. Now working at Adroit Systems, Alexandria, VA.

William Detlefs, M.S. (in Applied Math with Thesis) 1991.

Thesis: Longitudinal Coupling Impedance of a Thin Iris Collimator.

Employment: Now a graduate student with support in Physics at Cal Tech.

2.6 Other Students

Eric N. Opp (1984-85)

Spent one year working on the development of a computer program to calculate dispersions curves for azimuthally symmetric modes in an azimuthally symmetric periodic chain of coupled cavities. Now has earned Ph.D. in Plasma Physics.

Dimitris Vassiliadis (1987-88)

Spent 1 1/2 years working as a Graduate Research Assistant on Alternating Phase Focussing. Now has earned Ph.D. in a group working on chaos.

Jeffrey Skibo (1988-89)

Spent one year exploring possible further work on the use of Lie algebraic methods in the treatment of space charge. Also responsible for general computational support. Now has earned Ph.D. in High Energy Astrophysics.

Eric Salter (1990-91)

Spent one year working on the calculation of the impedance of a thick iris. Also did programming for MARYLIE and provided general computational support. Now serving as a Teaching Assistant.

Glenn VanderWoude (1988-1992)

Undergraduate student and National Merit Scholar. Responsible for general computational support. Now holds a Fellowship in Applied Mathematics at the State University of New York (Stony Brook) where he is pursuing graduate work for the Ph.D.

2.7 Past Ph.D. Professional Staff

Herbert O. Moser (1985)

Visiting Scientist, supported by German Government. Permanently at IMM Institut für Mikrotechnik, Mainz Germany.

Hiromi Okamoto (1989-90 and 1992-93)

Visiting Scientist, partially supported by Japanese Government. Permanently at Nuclear Science Laboratory, Institute for Chemical Research, Kyoto Japan.

Filippo Neri (1983-90)

Postdoctoral Research Associate. Presently at Los Alamos National Laboratory.

Fernando Casas (1992-1993)

Visiting Postdoctoral Fellow, supported by Spanish Government.

Branislav Radak (1992-1993)

Postdoctoral Research Associate.

Johannes van Zeijts (1987-1993)

Postdoctoral Research Associate. Presently at Continuous Electron Beam Accelerator Facility.

Ivan Gjaja (1991-1994)

Postdoctoral Research Associate and SSC Fellow. Will join the Center for Nonlinear Studies at the Los Alamos National Laboratory.

3 Research Accomplishments

Several of the objectives set forth in the 1992 proposal have been met, and additional objectives have been achieved as well. A brief summary of work accomplished over the last year is given below.

3.1 Task A: Charged Particle Beam Transport

1. The program MARYLIE 3.0, comprising approximately 32,000 lines of code, is nearly ready for wide distribution and general use. A detailed instruction manual, consisting of some 475 pages and set in TEX, is substantially complete.¹ Preliminary versions of the code have been tested on VAX, CRAY, IBM, SUN, and UNIX computers, and are in use in 30 Universities, Government Laboratories, and Industrial Companies in the United States, Canada, Europe, and Japan. The use of Lie algebraic methods and MARYLIE has been taught as part of the subject matter in the Summer 1993 and Summer 1994 U.S. Particle Accelerator Schools.
2. Continued improvements are being made in MARYLIE 3.0. Work is currently being done on optimizing routines. These routines adjust parameters to optimize arbitrary merit functions, and are of use when fits are not possible. New optimizers include genetic algorithms and the downhill simplex method.
3. A version of MARYLIE 3.1, a third-order code including error effects, has been assembled. The computation of error effects in nonlinear Hamiltonian systems using Lie algebraic methods has been worked out in detail, and applied to the problem of steering magnets and mispowered dipoles.² These computations have been implemented in MARYLIE 3.1.
4. Programming has continued on MARYLIE 5.1, a fifth-order code including error effects. Recent work shows that long-term tracking studies for large proton storage rings can be made using a fourth-order one-turn map and a generating function symplectification scheme.^{3,4} This method is orders of magnitude faster than element by element

tracking, and will permit much more detailed study of the anticipated performance of the LHC. All aspects of this method (production and use of a one-turn map and generating function symplectification) were originally conceived and developed at Maryland.^{5,6,7} MARYLIE 5.1 already implements these methods fully and should be an ideal code for LHC studies.

5. Work has continued on writing an extensive set of Lecture Notes on Nonlinear Dynamics and Lie Methods with Applications to Accelerator Physics.⁸ These Lecture Notes describe in detail results obtained previously, and also contain important new results. One of these new results is the introduction of a $U(3)$ and $USp(6)$ invariant scalar product in the vector space of Lie generators f_n .
6. The use of Taylor series maps to describe charged particle beam transport raises at least two questions. First, what is the domain of convergence of the series? Second, how can a truncated expansion be "completed" to be made symplectic? Work has begun on the first question as part of the thesis research of Dan Abell, and results have been found for the anharmonic oscillator.⁹ This work requires extensive use of the theory of several complex variables and leads to remarkable results. For example, the Hamiltonians $H = (p^2 + q^2)/2 \pm q^4$ both lead to Taylor maps having identical convergence domains.
7. Work on the second question in item 6 above began with the use of generating functions.^{5,6,7} Subsequently Irwin proposed a method that led to Cremona maps.¹⁰ Dragt, Rangarajan, Gjaja, and Abell continue to work on Cremona map and solvable map approaches.^{11,12,13,14,15} Some of this work was described in an invited talk presented at the 1992 Brookhaven Workshop on the Stability of Particle Motion in Storage Rings, and some is expected to be part of the thesis research of Dan Abell. Recently, significant advances have been made in the construction of Cremona maps. These advances include the following concepts:
 - (a) A careful discussion of what is required for a satisfactory symplectic completion.
 - (b) Use of the invariant scalar product described in item 5 above.⁸

- (c) The introduction of “sensitivity” vectors, the Gram matrix formed from them, and the demonstration that the quality of a Cremona map as a symplectic completion is related to the size of the smallest eigenvalue of the Gram matrix.
- (d) Explicit calculation of all the eigenvalues of the Gram matrix in the continuum limit, and the demonstration that these results are the best that can be hoped to be achieved.
- (e) Explicit construction of an optimal Cremona map for which the associated Gram matrix has these optimal eigenvalues. This construction made extensive use of the optimizers described in item 2 above.

Items a, b, and c above are described in a recent publication.¹⁶ Items d and e make use of new group-theoretic and quadrature-formula related results that will be described in subsequent publications and the thesis of Dan Abell.

- 8. Sufficient conditions have been derived for the convergence of the infinite product of Lie transformations that arises in the description of an arbitrary analytic nonlinear map.¹⁷ Work continues on relating this result to the conditions for convergence of Taylor series maps.
- 9. A Lie algebraic formulation of light ray optics has been developed earlier.^{18,19} This work has now been extended to the case of light wave optics including interference effects. A lengthy publication on this subject is in preparation.²⁰
- 10. A Lie algebraic description of charged particle beam transport including space charge effects has been developed earlier.^{21,22} At that time it was difficult to make comparisons between Lie algebraic methods and traditional particle in cell methods due to cell particle population fluctuations. With the advent of massively parallel computers such as the CM5, it is now possible to run particle in cell codes with a very large number of particles, and thereby reduce particle population fluctuations within individual cells. In collaboration with Robert Ryne at Los Alamos, work has resumed on comparing Lie algebraic and particle in cell results.

11. General moment invariants have been found for linear Hamiltonian systems.^{12,23,24} This work generalizes the concept of emittance to the full six-dimensional phase space, and shows that there are three conserved *eigen emittances* (constructed from second-order moments) for general linear Hamiltonian systems. It also shows that there are an infinite number of invariants for such systems that can be constructed from third and higher-order moments. Based on the work just described, a general new theory has been developed for the description of beams in a full six-dimensional phase space.²⁵ This theory generalizes the usual Twiss beam envelope description (used for the earlier two-dimensional phase space description) by the introduction of *envelope matrices* and *eigen phase advances* in addition to the *eigen emittances* described above. The computation of eigen emittances, envelope matrices, and eigen phase advances has been made a standard MARYLIE command. It is expected that these new tools will facilitate the calculation and description of projected emittance growth due to linear cross couplings.²⁶ Recently, an independent and possibly more efficient procedure has been found for constructing the invariants described above.²⁷ Also, work has begun on constructing the invariants that determine the equivalence classes of the Lie generators f_n under the action of $Sp(6)$. The classification is complete for the f_2 , and work has begun on the f_3 and the f_4 .²⁸ It is expected that this information will be useful for the symplectification of maps and the construction of map normal forms as well as the classification and construction of moment invariants and moment normal forms.
12. Work has begun on the construction of moment invariants for nonlinear Hamiltonian systems. Functions of moments that remain invariant for an arbitrary nonlinear Hamiltonian system have been constructed. The existence of these moment invariants is entirely a consequence of the symplectic nature of the flow generated by Hamiltonian systems. These invariants may be of use in accelerator design, in the general area of charged particle beam transport, and in other areas of Hamiltonian dynamics.²⁹

3.2 Task B: Computation of Electromagnetic Fields and Beam-Cavity Interactions

1. Coupling Impedance of a Thick Iris

Equations were derived for calculation of the longitudinal and transverse impedance of an iris in a beam pipe. The equations were cast in a variational form and implemented in a well convergent computer program to calculate the impedance [a]. Limiting results were obtained for a large beam pipe radius corresponding to the configuration of a hole in a thick metal plate.

Corresponding equations have also been derived for periodic irises, and numerical implementation is well under way.

2. Penetration of Fields through Circular Holes in a Conducting Wall

We have constructed a variational formulation to obtain the field penetration through a circular hole when the wavelength is finite. In the process we have generalized the definition of polarizability and susceptibility for finite wavelength. Numerical implementation has been completed [b] for the dependence of the polarizability on wavelength, and work is well under way for the corresponding susceptibility. In addition, work has been completed on the penetration of fields through an elliptical hole [c], and has started on the penetration of fields through a rectangular hole, using non-mesh semi-analytic methods.

3. Halo Formation in High Current Ion Linacs

An analytic model has been proposed [d,e], for the development of a halo in a high current ion linac. The model consists of a non-linear resonant interaction between a coherent oscillation of the beam core (like the “breathing” mode) and individual particle oscillations. The model gives excellent agreement with simulations being performed by Wangler and Ryne at LANL, as well as others elsewhere.

4. Stability of a “Breathing” K-V Beam

All halo formation models show the features of the halo by starting with particles outside the core. The question of how these particles

get outside the core is not yet clear. Perhaps the high current beam is unstable to some type of perturbation. We have been able to explore the stability of a mismatched K-V beam in a "breathing" mode. In particular we show analytically that perturbations with non-uniform charge density can be unstable, just as they may be for a matched beam [f,g], but at lower values of current. We are presently exploring this parameter space.

5. Trapped Modes in Waveguides with Small Discontinuities

A single small discontinuity (enlargement or hole) in a smooth waveguide can result in the appearance of trapped electromagnetic modes with frequencies slightly below the waveguide cutoff frequencies [h]. The trapped modes produce sharp resonance peaks of the coupling impedance near the cutoff frequencies. The analysis has been extended to include many small discontinuities [i], where it is found that the effect depends sensitively on the distribution of these discontinuities.

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[c] B. Radak and R.L. Gluckstern, "PENETRATION OF ELECTROMAGNETIC FIELDS THROUGH AN ELLIPTICAL HOLE IN A WALL OF FINITE THICKNESS", to be published in IEEE Transactions on Microwave Theory and Techniques, about December 1994.

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