Program and Abstracts
Semiclassical & multiscale aspects of wave propagation
Heraklion, Greece
May 28 – June 1, 2012

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Preface

This volume contains the abstracts of the talks presented at the Semiclassical & multiscale aspects of wave propagation Workshop held at Heraklion, Greece, on May 28–June 1, 2012. The workshop has been organized under the auspices of the Archimedes Center for Modeling, Analysis and Computation (ACMAC) and the Department of Applied Mathematics at the University of Crete.

The aim of this workshop is to bring together scientists working on semiclassical and multiscale techniques, in order to investigate the role and interconnectivity of their tools in the modeling, analysis and computation of wave phenomena.

We would like to thank all contributors for submitting their abstracts and presenting their work at the workshop.

George N. Makrakis

Organizing Committee

George N. Makrakis (University of Crete, Greece)
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PROGRAM

Monday, May 28, 2012

9:30-12:30  Morning Session

Analysis and computation for the semiclassical limits of the nonlinear Schroedinger equations
Weizhu Bao

Fast Gaussian wavepacket transforms and Gaussian beams for the Schroedinger equation
Jianliang Qian

Shock wave chaos
Aslan Kasimov

Tuesday, May 29, 2012

9:30-12:30  Morning Session

Asymptotically correct finite difference schemes for highly oscillatory ODEs
Anton Arnold

Numerical study of Kadomtsev-Petviashvili equations
Christian Klein

Tailored finite point method for wave equation
Zhongyi Huang

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Semiclassical approximations for Hamiltonians with operator-valued symbols
Stefan Teufel

Semiclassical limit of quantum dynamics for singular and rough potentials
Ioannis Giannoulis

Evolution of a point-supported Wigner measure under a potential with BV derivatives
Agis Athanassoulis
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9:30-13:30 Morning Session

- How do coherent states spread? Time evolution on Ehrenfest time scales
  Roman Schubert
- Interaction of coherent states for Hartree equations
  Remi Carles
- Semiclassical wave packets in periodic potentials
  Christof Sparber
- Wavepacket representation of semiclassical time evolution
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- Scattering problems for symmetric systems with dissipative boundary conditions
  Vesselin Petkov
- Stability estimate of stiffness from MRE data
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- Carleman estimates and anisotropic inverse problems
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2:15-17:30 Afternoon Session

- The mathematics of multiwave imaging
  Plamen Stefanov
- Schrodinger waves: interference and decoherence in experiment and simulation
  Norbert Mauser
- Singular semiclassical approximations
  Thierry Paul

Friday, June 1, 2012

9:30-12:30 Closing Session

- Discussions and directions of future research
ABSTRACTS

Analysis and computation for the semiclassical limits of the nonlinear Schroedinger equations

Weizhu Bao
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In this talk, I will review recent results on analysis and efficient computation for the semiclassical limits of linear and nonlinear Schroedinger (NLS) equations. First, I will show our recent asymptotic and numerical results on the semiclassical limits of the ground and excited states of time-independent NLS with a few typical external trapping potentials. Then I will review the formal semiclassical limit of the NLS by using different approaches including WKB method, Winger transform, Grenier's generalized WKB analysis, etc. A time-splitting spectral (TSSP) method was introduced to efficiently compute the dynamics of the NLS in the semiclassical regimes. The numerical method is explicit, unconditionally stable, time reversible and time transverse invariant. Moreover, it conserves the position density in the discretized level and has the best spatial/temporal resolution for the NLS in the semiclassical regimes. Comparison between the solutions of the NLS and its quantum hydrodynamical limit are presented, especially when the quantum hydrodynamical equations have shocks and/or vacuum. Finally, the analysis and computation results are extended for the NLS with an angular momentum rotation term and coupled nonlinear Schroedinger equations.

Fast Gaussian wavepacket transforms and Gaussian beams for the Schroedinger equation

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We introduce a wavepacket-transform-based Gaussian beam method for solving the Schroedinger equation. We focus on addressing two computational issues of the Gaussian beam method: How to generate a Gaussian beam representation for general initial conditions and how to perform long time propagation for any finite period of time. To address the first question, we introduce fast Gaussian wavepacket transforms and develop on top of them an efficient initialization algorithm for general initial conditions. Based on this new initialization algorithm, we address the second question by reinitializing the beam representation when the beams become too wide. Numerical examples in one, two, and three dimensions demonstrate the efficiency and accuracy of the proposed algorithms. The methodology can be readily generalized to deal with other semi-classical quantum mechanical problems.

Shock wave chaos

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We propose a simple model equation that describes chaotic shock waves. The equation is a modification of the Burgers equation that includes non-locality via the presence of the
shock-state value of the solution in the equation itself. The model predicts steady-state solutions, their instability through a Hopf bifurcation, and a sequence of period-doubling bifurcations leading to chaos. This is similar to the dynamics of detonations in the one-dimensional reactive Euler equations. We present nonlinear numerical simulations, complete linear stability theory for the model equation, and compare them to the solutions of the reactive Euler equation.

Asymptotically correct finite difference schemes for highly oscillatory ODEs
Anton Arnold
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We are concerned with the numerical integration of ODEs of the form $\epsilon^2 \psi_{xx} + a(x)\psi = 0$ for given $a(x) \geq \alpha > 0$ in the highly oscillatory regime $0 < \epsilon \ll 1$ (appearing as a stationary Schrödinger equation or 1D Helmholtz equation, e.g.). In two steps we derive an accurate finite difference scheme that does not need to resolve each oscillation: 1) With a WKB-ansatz the dominant oscillations are "transformed out", yielding a much smoother ODE. 2) For the resulting oscillatory integrals we devise an asymptotic expansion both in $\epsilon$ and $\hbar$. In contrast to existing strategies, the presented method has (even for a large spatial step size $\hbar$) the same weak limit (in the classical limit $\epsilon \to 0$) as the continuous solution. Moreover, it has an error bound of the order $O(\epsilon^2 \hbar^2)$. We shall give applications to k.p-Schrödinger systems and to the simulation of semiconductor-nanostructures. Ref: A. ARNOLD, N. BEN ABDALLAH and C. NEGULESCU: WKB-based schemes for the oscillatory 1D Schrödinger equation in the semi-classical limit, SIAM J. Numer. Anal. 49, No. 4 (2011) 1436-1460. J. GEIER, A. ARNOLD: WKB-based schemes for two-band Schrödinger equations in the highly oscillatory regime, Nanosystems: Physics, Chemistry, Mathematics 2, No. 3 (2011) 7-28.

Numerical study of Kadomtsev-Petviashvili equations
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We present a numerical study of the Kadomtsev-Petviashvili (KP)equations. First we study the stability of exact solutions to the Korteweg-de Vries equation, the soliton and the cnoidal traveling wave solution within the KP framework. Then we study the stability of exact solutions to the KP equation. The small dispersion limit of the KP equation as well as the singularity formation of solutions in the dispersion-less KP equation are addressed numerically. Finally we investigate the question of blow-up in generalized KP equations.

Tailored finite point method for wave equation
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In this talk, following the idea of the tailored finite point method proposed in our former papers, a series of efficient numerical schemes are developed for the one dimensional scalar wave equation within various types of media. Stability and accuracy are analyzed.
and numerically verified. In particular we can obtain unconditionally stable implicit schemes that can be solved explicitly for boundary value problems. We can also deal with the propagation of discontinuity and highly oscillatory waves efficiently. The generalization to higher order schemes is straightforward. It is a joint work with Dr. Xu Yang.

### Semiclassical approximations for Hamiltonians with operator-valued symbols

Stefan Teufel  
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I present a simple but rigorous derivation and justification of the semiclassical model for the slow degrees of freedom in adiabatic slow-fast systems. It is shown that it approximates stationary quantum mechanical expectations and the time-evolution of operators also in sub-leading order in the combined adiabatic and semiclassical limit. In the context of Bloch electrons the semiclassical model has led to substantial progress during the recent years.

### Semiclassical limit of quantum dynamics for singular and rough potentials

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We present results of joint work with L. Ambrosio, A. Figalli, G. Friesecke, and T. Paul concerning the rigorous justification of classical molecular dynamics as the semiclassical limit of quantum dynamics, where the potential of the Schrödinger equation is given by the Born-Oppenheimer potential energy surface. While the Coulombic terms of the potential can be treated with in a rather "classical" weak sense, its roughness, originating from eigenvalue crossings, allows only for the justification of classical dynamics for "almost all" initial data.

### Evolution of a point-supported Wigner measure under a potential with BV derivatives

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How do coherent states spread?  
**Time evolution on Ehrenfest time scales**

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We derive an extension of the standard time dependent WKB theory which can be applied to propagate coherent states and other strongly localized states for long times. It
allows in particular to give a uniform description of the transformation from a localized coherent state to a delocalized Lagrangian state which takes place at the Ehrenfest time.

The main new ingredient is a metaplectic operator which is used to modify the initial state in a way that standard time dependent WKB theory can then be applied for the propagation.

Interaction of coherent states for Hartree equations

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We consider the Hartree equation with a smooth kernel and an external potential, in the semiclassical regime. We analyze the propagation of two initial wave packets and show different possible effects of the interaction, according to the size of the nonlinearity in terms of the semiclassical parameter. We describe precisely different sorts of nonlinear phenomena.

Semiclassical wave packets in periodic potentials

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We consider semi-classically scaled (weakly nonlinear) Schroedinger equations with an external potential and a highly oscillatory periodic potential. We construct asymptotic solutions in the form of semiclassical wave packets, i.e. coherent states propagating within a given Bloch energy band. These solutions are concentrated (both, in space and in frequency) around the effective semiclassical phase-space flow and involve a slowly varying envelope whose dynamics is governed by a homogenized Schroedinger equation with time-dependent effective mass. In the linear case, the corresponding adiabatic decoupling of the slow and fast degrees of freedom is shown to be valid up to Ehrenfest time scales. (Joint work with R. Carles).

Wavepacket representation of semiclassical time evolution

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Scattering problems for symmetric systems with dissipative boundary conditions

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To build a scattering theory for symmetric systems with dissipative boundary conditions one constructs the wave operators $\mathcal{W}_1(\pm)$ related to the asymptotic profiles for $t \to \pm \infty$. The boundary problem determines a contraction semigroup $V(t) = e^{\tau G}$. 

ACMAC/SMAW2012
Stability estimate of stiffness from MRE data

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MRE (magnetic resonance elastography) is a new diagnosing modality to measure stiffness of human tissues by MRI combined with a vibration system. MRE can give an image of waves generated by the vibration system. Then, via some pde model, the identification of the stiffness becomes a coefficient identification inverse problem of the pde model by knowing a solution of this pde. In this talk a Holder stability estimate will be presented for the so called scalar pde model for MRE by assuming that the coefficients of this pde model is piecewise analytic.

Carleman estimates and anisotropic inverse problems

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Calderón’s inverse problem is whether one can uniquely determine the electric conductivity of an object by making boundary measurements. A geometric formulation of the anisotropic version of this problem is whether it is possible to recover a compact Riemannian manifold with boundary from the Cauchy data of harmonic functions. The problem is well understood in dimension two and in the analytic category but remains challenging for smooth manifolds in dimension higher than three. The recent developments in the case of conformal metrics are based on Sylvester and Uhlmann’s approach for the isotropic case and rely heavily on Carleman estimates and construction of harmonic functions by complex geometrical optics.

The mathematics of multiwave imaging

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We will review the recent theoretical and numerical results obtained together with G. Uhlmann, J. Qian and H. Zhao on thermoacoustic and photoacoustic tomography in medical imaging. The model is the wave equation with a variable speed in the whole space, with measurements taken on a (part of) a boundary, invisible to the waves. The results include necessary and sufficient condition for uniqueness and for stability for partial boundary, a Neumann series type of reconstruction formula for full boundary, and
a microlocal characterization of the data. We also study a piecewise smooth speed modeling brain imaging. Numerical reconstructions will be presented as well.

**Schroedinger waves : interference and decoherence in experiment and simulation**

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**Singular semiclassical approximations**

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I will review some recent results concerning the subject.