Summer School *“Around Schrödinger”*
3-7 August, 2015

WPI seminar room, 8^{th} floor, Fak. Mathematik, Univ. Wien
Oskar MorgensternPlatz 1, 1090 Wien

Monday 3. Aug

14h00 : Norbert J **Mauser** (WPI & ICP c/o U. Wien)
“Welcome to Vienna, birthplace of Boltzmann, Schrödinger and Pauli”

14h15 : Yann **Brenier** (CNRS X):
"When Madelung comes up...."

15h15 : Pierre **Germain** (Courant)
“On the derivation of the kinetic wave equation”

Tuesday 4. Aug

10h00 : Francois **Golse** (X) :
“On the mean-field and classical limits for the N-body Schrödinger equation”

11h00 Francis **Nier** (U.Paris 13):
“*Phase-space approach to the bosonic mean field dynamics : a review”*

12h00 Boris **Pawilowski** (U.Wien & U. Rennes):
“Mean field limits for discrete NLS: analysis and numerics”

14h00 Toan **Nguyen** (Penn State):
"Grenier's iterative scheme for instability and some new applications".

Wednesday 5. Aug

10h00 : Alex **Gottlieb** (WPI):
“Entropy measures for quantum correlation”

11h00 Claude **Bardos** (WPI & ICP c/o Paris):
“Formal derivation of the Vlasov Boltzmann relation”

12h00 Hung **Luong** (U. Wien):
“On the Cauchy problem of some 2-d models on the background of 1-d soliton solution of the cubic nonlinear Schrödinger equation"

Thursday 6. Aug

10h00 : Christophe **Besse** (U.Toulouse):
“*Exponential integrators for NLS equations with application to rotating BECs“*

11h00 : Stephane **Descombes** (U.Nice):
“Exponential operator splitting methods for evolutionary problems and applications to nonlinear Schrödinger equations in the semi-classical regime“

13:30 Yong **Zhang** (WPI):
“Efficient evaluation of nonlocal potentials: NUFFT and Gaussian Sum Approximations”

14:30 Hans-Peter **Stimming** (WPI c/o U.Wien):
“Absorbing Boundary Conditions for Schrodinger and Wave equations: PML vs ECS”

Abstracts:

Yann **Brenier** (CNRS X):
"When Madelung comes up...."

After recalling the remarkable formulation made in 1926 by Erwin Madelung of the Schrödinger equation in terms of fluid mechanics, I will introduce a rational scheme, based on the least action principle and some non-linear rescaling of the time variable, starting from Euler's equations of isothermal compressible fluids (1755), followed by Fourier's heat conduction equation (1807), leading to Schrödinger's equation of quantum mechanics (1925).
Finally, I will suggest the application of this scheme to Magneto-hydrodynamics.

Madelung, E. (1926). "Eine anschauliche Deutung der Gleichung von Schrödinger". *Naturwissenschaften* **14** (45): 1004–1004.

Pierre **Germain** (Courant)
“On the derivation of the kinetic wave equation”

The kinetic wave equation is of central importance in the theory of weak turbulence, but no rigorous derivation of it is known. I will show how it can be derived from NLS on the torus with random forcing, in the small nonlinearity / big box limit. This is joint work with Isabelle Gallagher and Zaher Hani.

Francois **Golse** (X) :
“On the mean-field and classical limits for the N-body Schrödinger equation”

This talk proposes a quantitative convergence estimate for the mean-field limit of the N-body Schrödinger equation that is uniform in the classical limit.
It is based on a new variant of the Dobrushin approach for the mean field limit in classical mechanics, which avoids the use of particle trajectories and
empirical measures, and has a very natural quantum analogue. (Work in collaboration with C. Mouhot and T. Paul).

Francis **Nier** (U.Paris 13):
***“**Phase-space approach to the bosonic mean field dynamics : a review”*

After recalling old or more recent point of views on bosonic quantum field theory and mean field problems, the series of works in collaboration with Z. Ammari will be summarized. This phase-space presentation implements the old dream of an infinite dimensional microlocal analysis. In particular the mean field dynamics is nothing but a propagation of singularity result in the semiclassical regime. This talk will put the stress on the key issues related with the infinite dimensional setting and on the new results for the mean field problem provided by this approach.

Boris **Pawilowski** (U.Wien):
"Mean field limits for discrete NLS: analysis and numerics"

In my thesis, jointly supervised by N.J. Mauser and F. Nier, we deal with approximations of the time-dependent linear many body Schrödinger equation with a two particles interaction potential, by introducing a discrete version of the equation and mean field limits.
We consider the bosonic Fock space in a finite dimensional setting.
Mathematical tools include the reduced density matrices and Wigner measure techniques exploiting the formal analogy to semi-classical limits.

Toan **Nguyen** (Penn State):
"Grenier's iterative scheme for instability and some new applications".

"The talk is planned to revisit Grenier's scheme for instability of Euler and Prandtl, introduced in his CPAM-2000 paper, and to present some new applications in the instability of generic boundary layers and instability of Vlasov-Maxwell in the classical limit".

Alex **Gottlieb** (WPI):
"Entropy measures for quantum correlation"

We use quantum Rényi divergences to define "correlation" functionals of many-fermion states (density operators on a Fock space).
The "reference" state for the relative entropy functional is the unique gauge-invariant quasi-free (g.i.q.f.) state with the same 1-RDM as the state of interest.
That is, the "correlation" of the state of interest is its Rényi divergence from the uniquely associated g.i.q.f. state.
Correlation functionals defined in this way enjoy the following properties:
(a) they take only non-negative values, possibly infinity;
(b) they assign the value 0 to all Slater determinant states;
(c) they are monotone with respect to restriction of states;
(d) they are additive over independent subsystems;
and
(e) they are invariant under changes of the 1-particle basis (Bogoliubov transformations).

The quantum relative entropy or quantum Kullback-Leibler divergence is a special and distinguished member of any family of quantum Rényi divergences (of which there are at least two).
The associated correlation functional, defined using quantum Kullback-Leibler divergence, we call "nonfreeness."
Nonfreeness enjoys further appealing properties not shared by related correlation functionals:
(f) the nonfreeness of a state X is the minimum possible value for the entropy of X relative to any g.i.q.f. reference state;
(g) there is a simple formula for a pure state's nonfreeness in terms of it's natural occupation numbers; and
(h) within the convex set of n-fermion states with given 1-RDM, the nonfreeness minimizer equals the entropy maximizer, which is the Gibbs canonical (n-particle) state.

Claude **Bardos** (WPI & ICP c/o Paris) :
"Formal derivation of the Vlasov Boltzmann relation"

I report on current work with Toan Nguyen and Francois Golse.

Hung **Luong** (U. Wien):
"On the Cauchy problem of some 2-d models on the background of 1-d soliton solution of the cubic nonlinear Schrödinger equation"

I present an overview about the transverse stability problem and some results on the Cauchy problems of Davey-Stewartson systems (a perturbation model of the nonlinear Schrödinger equations (NLS)). In the last part of my talk, I will briefly introduce some other models which are also a perturbation of NLS. This is a thesis in progress, jointly supervised by N.J Mauser and J.C. Saut.

Christophe **Besse** (U.Toulouse):
„Time integrators for NLS equations with application to rotating BECs"

In this talk, I will present various time integrators for NLS equations when the potentials are time dependent. In this case, the usual time splitting schemes fail. I will introduce exponential Runge-Kutta scheme and Lawson scheme and present some of their properties.

Stephane **Descombes** (U.Nice):
"Exponential operator splitting methods for evolutionary problems and applications to nonlinear Schrödinger equations in the semi-classical regime"

In this talk, I investigate the error behaviour of exponential operator splitting methods for nonlinear evolutionary problems. In particular, I will present an exact local error representation that is suitable in the presence of critical parameters. Essential tools in the theoretical analysis including time-dependent nonlinear Schrödinger equations in the semi-classical regime as well as parabolic initial-boundary value problems with high spatial gradients are an abstract formulation of differential equations on function spaces and the formal calculus of Lie-derivatives.

Yong **Zhang** (WPI):
"Efficient evaluation of nonlocal potentials: NUFFT and Gaussian Sum Approximations"

We introduce accurate and efficient methods for nonlocal potentials evaluations with free boundary condition, including the 3D/2D Coulomb, 2D Poisson and 3D dipole-dipole potentials. Both methods rely on the same assumption: the density is smooth and fast decaying. The first method,proposed by Jiang, Greengard and Bao, evaluates the potential in spherical/polar coordinates using NonUniform FFT algorithm, where the singularity of the Fourier representation disappears automatically, while the second one is based on a Gaussian-sum approximation of the singular convolution kernel and Taylor expansion of the density.
Both methods are accelerated by fast Fourier transforms (FFT). They are accurate (14-16 digits), efficient ($O(N\log N)$ complexity), low in storage, easily adaptable to other different kernels, applicable for anisotropic densities and highly parallelizable.

Hans-Peter **Stimming** (WPI c/o U.Wien):
"Absorbing Boundary Conditions for Schrödinger and Wave equations: PML vs ECS"

The perfectly matched layers (PML) and exterior complex scaling (ECS) methods for absorbing boundary conditions are analyzed using spectral decomposition. Both methods are derived as analytical continuations of unitary to contractive transformations. We find that the methods are mathematically and numerically distinct: ECS is complex stretching that rotates the operator's spectrum into the complex plane, whereas PML is a complex gauge transform which shifts the spectrum. Consequently, the schemes differ in their time-stability. Numerical examples are given.