## 2. Research goals and research methods

The main goal of this USP project is the development of mathematical models and computational methods and their application to computer simulations in collaboration with partners in quantum physics, quantum chemistry and quantum electronics. The similarities in mathematical structures of models in different application areas allow to develop new methods in a general setting. The 2 "main themes", Nonlinear Schrödinger equations and (quantum) Boltzmann equations are somewhat linked by "kinetic formulations" of PDEs and in particular by the Wigner transform that maps between the physical space of NLS (and macroscopic models like (quantum) fluid dynamics) and the "phase space" of kinetic equations. The inclusion of a "collision operator" in the Wigner equation, which yields what can be called "quantum Boltzmann equations" in the strict sense of kinetic equations, is a challenging long term goal both from the modeling and the numerical point of view.

The approximation of the numerically intractable linear "N-body Time Dependent Schrödinger" (N-TDS) equation by (systems of) nonlinear one-particle Schrödinger equations yields a large variety of models from the "Multi-Configuration Time Dependent Hartree-Fock" (MCTDHF) method to "Time Dependent Density Functional Theory" (TDDFT).

The particular research topics/goals are :

(i) Numerical analysis of MCTDHF, e.g. the proof of convergence of solutions of MCTDHF to solutions of N-TDS for increasing number of configurations with N fixed, related to the proof that this method has better convergence properties than a simple Galerkin method with fixed basis functions. Improved numerical algorithms for MCTDHF. Simulations for problems in photonics and quantum chemistry.

(ii) Numerical methods for TDDFT, including relativistic and current dependent TDDFT in models like the Dirac-Kohn-Sham system coupled to Maxwell equations. Simulations for problems in material science (e.g. ultrafast spectroscopy, magnetic switches).

(iii) Numerical simulations for NLS in various contexts
a) Simulation of Blow-up phenomena in focusing NLS
b) Bose-Einstein Condensates (Gross-Pitaevskii equation)
c) KP equations
d) Pushing the threshold in semiclassical computations for Schrödinger type equations, also using and comparing to WKB methods and Bloch decomposition methods.

(iv) The formulation and numerical simulation of quantum transport models including electron-phonon interaction which yields a class of "quantum Boltzmann equations". This involves a systematic simplification procedure starting from a full quantum mechanical description of the electron-phonon system including the influence of the crystal lattice. Also we shall deal with the numerics of approximate models like "quantum Fokker-Planck equations". The recent work on SHE models (Spherical Harmonic Expansions) related to quantum entropy models shall be exploited for improved numerical algorithms.

(v) Contribution to the development of efficient numerical approaches for kinetic transport models. In particular, stochastic particle methods based on cubature in path space could provide an improvement of standard Monte Carlo methods. The corresponding theory, recently developed for stochastic processes based on Brownian motion will be extended to Poisson jump processes.

As a method/tool for (i,ii, iii) it should be noted that the currently used simulation code for NLS, developed by Markowich, Bao and Jin (essentially a time splitting spectral method), has

been increasingly extended to a universal tool for all sort of generalized NLS. Stimming has developed a parallelized version performing very well on the Schrödinger II and III machines of the ZID of the Univ. Wien, allowing for semiclassical simulations in 3-d (up to 1000 gridpoints in each spatial direction).
Despite its advantages, however, this code shall be replaced by a new NLS solver (using adaptive grid redistribution) at the end of this project, including a parallelized version.

2.1. **ad (i) : MCTDHF.** It is an important problem in quantum physics and quantum chemistry to find numerically tractable approximations of the "exact" many-body problem of non-relativistic quantum dynamics of N interacting electrons (and M nuclei that we lump into the "external potential"). In the non-relativistic case one would ideally like to solve the N-body time-dependent linear Schrödinger equation (N-TDS) with Coulomb potential and a time-dependent external potential $V(\mathbf{r}_j, t)$, which reads

$$i\frac{\partial}{\partial t}\Psi \;=\; \sum_{j=1}^{N}\Big(-\tfrac{1}{2}\Delta_{\mathbf{r}_j}\Psi + V(\mathbf{r}_j,t)\Psi\Big) + \sum_{1\le j<k\le N} W(|\mathbf{r}_j-\mathbf{r}_k|)\Psi$$

in atomic units. Here $\Psi = \Psi(\mathbf{r}_1, \mathbf{r}_2, \ldots, \mathbf{r}_N)$, and $\mathbf{r}_j \in \mathbb{R}^3$ denotes the position coordinates of the $j^{th}$ particle. The binary interaction potential $W$ is typically given by the Coulomb potential $W(|\mathbf{r}_j - \mathbf{r}_k|) = \frac{C}{|\mathbf{r}_j-\mathbf{r}_k|}$.
Although (1) is a linear PDE, it scales computationally in an exponential way with increasing number of particles which makes it practically impossible to compute solutions directly for systems with more than very few electrons.

To avoid this problem, often (coupled systems of) nonlinear Schrödinger equations for several single-electron "orbitals" are used in practice. One way to obtain such simplified models from (1) is by "variational approximation". This technique produces the time-dependent Hartree-Fock (TDHF) or *multiconfiguration* time-dependent Hartree-Fock (MCTDHF) sytems, and large variety other possibilities [42]. A different approach is time-dependent density functional theory (TDDFT) which produces the time-dependent Kohn-Sham system [46] and [1].

To illustrate the variational method we consider the 2-particle MCTDHF-ansatz

$$\Psi(x_1,x_2) \;=\; \sum_{j,k=1}^{n} a_{jk}\phi_j(x_1)\phi_k(x_2), \tag{1}$$

where $\{\phi_1, \phi_2, \ldots, \phi_n\}$ is an orthonormal set of $n \ge 2$ spin-orbitals. The coefficients satisfy $a_{kj} = -a_{jk}$ so that $\Psi$ is antisymmetric, thus obeying Pauli's exclusion principle, and $\sum |a_{jk}|^2 = 1$ to ensure $\|\Psi\| = 1$.

The Dirac-Frenkel variational principle yields a system of ordinary differential equations for the coefficients $a_{jk}$, coupled to a system of partial differential equations for the spin-orbitals $\phi_i$ which reads in vector notation for $\vec{\phi} = (\phi_1, \phi_2, \ldots, \phi_n)^T$

$$\frac{d}{dt}a_{jk} = -i\Big\langle \phi_j(x_1)\phi_k(x_2), V\Psi(x_1,x_2)\Big\rangle \qquad \forall j,k \tag{2}$$

$$\frac{d}{dt}\vec{\phi} = \frac{i}{2}(\Delta\otimes I_n)\vec{\phi} - i((I-P)\otimes\Gamma^{-1}\overline{A})V_{\vec{\phi}}(\Psi)\ . \tag{3}$$

Here A is the antisymmetric coefficient matrix and $\Gamma = \overline{A}A^T$. $P$ is the projection onto the subspace spanned by the orbitals $\phi_i$, $V_{\vec{\phi}}(\Psi)$ denotes the vector $(V_{\phi_1}(\Psi), \ldots, V_{\phi_n}(\Psi))^T$, where

$V_{\phi_j}(\Psi)$ is defined by

$$\langle \xi, V_{\phi_j}(\Psi) \rangle = \int \overline{\xi(x_1)\phi_j(x_2)} V(x_1, x_2)\Psi(x_1, x_2) dx_1 dx_2$$

To calculate numerical solutions of the MCTDHF equations is not trivial, since it requires the solution of a nonlinear system of ODEs for the coefficients $a_{jk}(t)$ coupled to the evolution equations for the "orbitals" $\phi_i(\mathbf{r}, t)$.

In order to solve the MCTDHF equations (as well as the TDHF equations) we currently use the time-splitting spectral scheme which was originally developed for the cubic NLS [2] and which has been proven to be a very efficient tool for very general classes of NLS (e.g. [1], [9]).

Using Born von Karman periodic boundary conditions on a sufficiently large domain of calculation fits well with the trigonometric spectral method for the free evolution that is split in time from the nonlinear potential part that yields an ODE that is solved by a fourth order Runge-Kutta scheme.

Clearly, these methods are far from being optimal. Our goal for MCTDHF is to develop new efficient numerical methods for the solution of system of equations like (2), (3) and to perform numerical tests to study systematically how the (MC)TDHF models perform in the context of computationally feasible simple problems, compared to the linear N-particle Schrödinger equation.

It is basically impossible to estimate "a priori" which of the models in the hierarchy is "better" for the calculation of a certain quantity - for example it is well known that sometimes the simple Hartree approximation gives better results than the more sophisticated Hartree Fock equation, especially when "correlation" effects play a role that are ignored by definition in the TDHF method. (cf e.g. [5] and [25]).

Clearly, MCTDHF is the canonical way to improve the TDHF method and should, with increasing number of configurations, converge to the solutions of the N-SE.

Let us remark that for MCTDHF many basic mathematical questions are open, starting with existence of unique global solutions for the Coulomb case (cf. [35], [59], [6]) because of an intrinsic problem of loss of rank of the density matrix after finite time (cf a interesting related recent result on "low rank approximations" of Lubich et al. [36]. Such analytical studies will have importance for the numerical algorithms.

2.2. **ad (ii) : TDDFT.** Density functional theory is a different (but related) approach to replace (1) by simpler nonlinear "one particle" models. It consists of approximating (1) by a system of electrons with self-consistently determined potential fields which model the interactions. Time-dependent density functional theory (TDDFT) is based on analogues of the fundamental Hohenberg-Kohn Theorem and variational principle that were first expounded in [54] and leads to the time-dependent Kohn-Sham system

$$i\frac{\partial}{\partial t}\phi_j(x,t) = \left[-\tfrac{1}{2}\Delta + V_{KS}[\rho](x,t)\right]\phi_j(x,t) \qquad (4)$$
$$j = 1, 2, \ldots, N$$

where the Kohn-Sham potential is defined as

$$V_{KS}[\rho](x,t) = V_0(x,t) + V_H[\rho](x,t) + V_{XC}[\rho](x,t) \ ,$$

and the density $\rho(x,t)$ depends on the Kohn-Sham orbitals $\rho(x,t) = \sum_{j=1}^{N} |\phi_j(x,t)|^2$ . Here $V_0$ is an external potential, $V_H[\rho](x,t)$ is the Hartree interaction potential and $V_{XC}[\rho](x,t)$ is the exchange-correlation potential.

One of the principal weaknesses of DFT as such is that the functional $V_{XC}[\rho]$ is generally unknown, and one is forced to make a heuristic ansatz (based on a guess more or less guided by insight into the physics) to be plugged into (4). For the time dependent case the functional depends also on the initial data - i.e. in general for each different initial density matrix a different functional is necessary. Moreover, the unknown dependence of $V_{KS}[\rho(\cdot,\cdot)](x,t)$ on the time-dependent density $\rho(x,t)$ is probably very complicated : Causality of $V_{KS}$ can be assured by deriving $V_{KS}$ from a proper action functional, but $V_{KS}$ will still be nonlocal in time and space ([24]).

In the stationary theory, the following formulations exist today:

- basic DFT for time-independent, non-relativistic system yielding $V_{XC}[\rho](x)$
- spin polarized density functional theory with the density $n(\mathbf{r})$ and the magnetization density $\mathbf{m}(\mathbf{r})$ as basic quantities.
- Current density functional theory which still uses a Schrödinger-type Hamilton operator but considers the density and the current density operators as the fundamental quantities
- A relativistic density functional theory (RDFT) using the Kohn-Sham-Dirac equations, here there are open questions remaining about an approximative form of the Dirac equation which couples the magnetic field to the spin current only. This approximation is widely used in physics but recently has been criticized for its missing terms to be more relevant. For the general form of the Kohn-Sham-Dirac equation there are still questions remaining regarding the use of a proper XC functional for the vector potential.

In the time-dependent theory the choice of the appropriate functional is largely open, but there are as well some already developed methods. One of our goals is to perform reliable numerical simulations for a detailed comparison of the different already existing TDDFT "exchange-correlation functionals" in order to obtain further insight in the applicability of TDDFT to various physical problems. For the case of spin polarized DFT, current DFT, or even relativistic DFT, new functionals have to be found and applied.

A simulation code for Nonlinear Schrödinger type equations exists already [1] which is applicable to a wide family of model equations. An extensive adaptation of the algorithm is necessary to include magnetic fields and the Spin-dependent cases. The artificial boundary conditions present problems for unstable simulations and some other treatment than the Born-Von Karman method will be needed, for example a PML-method.

In the long term it will be necessary to employ geometry-specific Multi-Grid methods to enhance performance and accuracy of simulations.

An important task is the extension of the above described mean field quantum models like TDHF to the **"relativistic regime"**. This includes both relativistic corrections to the TDDFT/TDHF equations as well as a fully relativistic setting relying on nonlinear Dirac type models. The numerical treatment of such systems is itself a notable task. Quite recently scientific progress has been achieved in this area: On the one hand several analytical results concerning asymptotic limits of the so-called "Maxwell-Dirac system" have been achieved by the proponents of this USP in [11, 14, 39, 56]. This is a mean field system replacing the classical Hartree (-Fock) model

by

$$(5)\qquad \begin{cases} i\partial_t\psi = \sum_{k=1}^{3} \alpha^k \left(-i\partial_{x_k} - (A_k + A_k^{ex})\right)\psi + q(V + V^{ex})\psi + mc^2\beta\psi, \\ (\partial_{tt} - \Delta_x)\, V = |\psi|^2, \quad (\partial_{tt} - \Delta_x)\, A_k = \overline{\psi}\cdot(\alpha^k\psi), \quad k = 1,2,3, \end{cases}$$

i.e. a nonlinear Dirac equation for the electron-positron 4-spinor, coupled to the Maxwell system for the self-consistent (electromagnetic) fields $V, A_k$. Additionally one may take into account external electromagnetic potentials $V^{ex}, A_k^{ex}$. Additionally to the above mentioned analytical studies there is recent work of Markowich, Sparber et al. on a numerical treatment of this system in [29]. We plan to adapt the code of [29] for the use on parallel architecture and extend it to include a Kohn-Sham-Dirac system.

The main drawback of the Maxwell-Dirac system is its lacking rigorous derivation of an underlying quantum field theory of electrodynamics. Indeed one may argue that the Maxwell-Dirac system should better be replaced by the so-called "Bogoliubov-Dirac-Fock system". This model has been recently derived from first principles in [33] and further studied in [30, 31, 32]. It provides a more natural description of the electrons and positrons as well as their (self-consistent) interactions (in Coulomb Gauge). Moreover, interaction with the vacuum background is taken into account and one is provided a positive definite energy functional, an important advantage in comparison to the Maxwell-Dirac system. Finally it is known that the non-relativistic limit of the Bogoliubov-Dirac-Fock system yields the above mentioned Hartree-Fock equations, which clearly provides a first link between this relativistic systems and the more classical mean field models based on Schrödinger type equations, as it has been obtained for the "simple" Dirac-Maxwell model by Mauser et al. [13, 14].

2.3. **ad (iii): NLS.** This is somewhat the central topic of this project where we deal with several classes of NLS type equations and applications in different contexts, partly connected to topic (ii) and (iv) :

**a) Simulation of "blow up" phenomena of NLS**
Consider the following class of focusing NLS:

$$i\partial_t u + \Delta u = -\lambda|u|^{2\sigma}u\ , \quad u_{|t=0} = u_0\,.$$

A local nonlinearity as in this equation appears in DFT models like, for example, the Schrödinger-Poisson-X$\alpha$ equation.
It is well known that if $\sigma \geq \frac{2}{n}$, a $H^1$-solution may blow up in finite time $T^*$, i.e. $\|u\|_{H^1} \to \infty$ for $t \to T^*$, hence no existence for $t \geq T^*$. This phenomenon is a source of many open questions, and research on this field has been going on for a long time, with some recent breakthroughes from the analysis point of view (F. Merle et al), (see for example [53], [58], [50]) yet many questions are still open. It is known that $L^2$-concentration takes place at blowup, i.e. positive $L^2$-mass concentrates at a finite set of points or a zero measure set. Most of the theoretical effort so far has been put on the question of self similarity, and finding possible blow-up profiles and blow-up rates. The "Townes Soliton" has long been known to be a possible blow-up profile. Recently it has been shown that blow-up is also possible on a ring-shaped profile [23]. Self-similar solutions known so far are unstable in general, and consequently also the related blow-up rates.

On the other hand little is known about the time $T^*$ at which blow-up occurs and ways to relate it, for example, to parameters in the equation and initial data. In fact, this question *when* the blow-up starts is much more interesting for the applications than the precise blow-up

profile. Since analytical results are mostly out of reach, this problem of studying blow-up times numerically (and phenomena like "multiple blow-up") is one of the most interesting problem of scientific computing in the field of NLS. To have reliable simulations is interesting both for applications and for the advancement of the theory. Current numerical studies of blow-up led by the proponents [10] are very promising. They show that in contrast to common conjectures the blow-up time does not decrease monotonously with respect to a varying scale $\lambda$ of the nonlinear term. The simulations are verified by comparison of simulations with two completely different codes: the time splitting spectral scheme developed in Vienna and a finite difference relaxation method developed in Toulouse/Lille.

New adaptive methods are necessary in order to also resolve the blow up profiles. The Blow-Up "Lens" transform [44], for example, is reliable close to blowup, but it is not clear what happens away from blowup and it is not possible to treat multi-point blowup with this method. A self-adaptive grid refinement would be a very promising approach, the drawback there is that this does not allow for application of other than the most simple , i.e. explicit, numerical methods for the equations.

Further numerical studies are needed e.g. to understand interaction of self-focusing with dispersing or other effects and to address questions like finding a priori blow-up times and "places". Furthermore one would like to know if other geometries than points or circles are possible. Also it would be interesting to quantify for given data how much of the $L^2$-charge will enter into collapse. In this context a most interesting point is the possibility to continue the part of the solution that does not collapse after the blow-up time, in the spirit of [17].

**b) PDE Models of Bose Einstein Condensates**
In the context of NLS models for Bose-Einstein distributions several results, aiming in different directions, have been achieved by the proponents. On the one hand the rigorous derivation of lower dimensional NLS in situations where there is a strong confinement in one or two dimensions are given in [8] and numerically studied in [4] (in the latter work one allows for more general initial data). The situation of BECs in so-called "optical lattices", modeled by a periodic potential, i.e.

$$i\partial_t\psi = -\frac{1}{2}\Delta\psi + V(x)\psi + U(x)\psi + \alpha|\psi|^2\psi, \quad \alpha \in \mathbb{R}, \tag{6}$$

where $V(x+\gamma) = V(x)$, $\forall x \in \mathbb{R}^3$, $\gamma \in \Gamma \simeq \mathbb{Z}^3$ (the lattice), is addressed in [19] and [55]. To this end rigorous semi-classical asymptotics and effective mass theorems are established, the latter yielding an equation of the form

$$i\partial_t f = -\frac{1}{2}\,\mathrm{div}(M^*\nabla)f + U(x)\psi + \kappa^*\,|f|^2 f, \tag{7}$$

as used in the physics literature (see [52]). Here we denote by $M^* = D_k^2 E_n(k_0)$, the effective mass tensor, i.e. the Hessian matrix of the $n$th Bloch energy band $E_n(k)$, $n \in \mathbb{N}$, induced by the lattice potential $V$, $\kappa^* \in \mathbb{R}$ is an effective coupling constant and $U$ some given non-periodic (possibly confining) potential.

Also a new numerical algorithm to study such problems, i.e. (linear) Schrödinger type equations with periodic potentials is proposed in [28]. It is shown there, that this new Bloch-decomposition based algorithm is superior to the standard time-splitting schemes in the sense that the same accuracy can be achieved using much fewer time-steps and a coarser spatial grid. As a follow-up work we currently extend this new numerical method to nonlinear Schrödinger equations too, focusing on nonlinearities of different strength in particular.

**c) KP equation**
A new branch of research which is connected to the above has been started in [34]. There a nonlinear dispersive wave equation, namely the "Kadomtsev-Petviashvili equation"(KP) is studied numerically. This $2+1$ dimensional equation, given by

$$\partial_x(\partial_t u + u\,\partial_x u + \partial_{xxx} u) + \lambda\,\partial_{yy} u = 0, \quad \lambda = \pm 1, \tag{8}$$

is formally obtained as a model for matter wave pulses in BECs as well as for sound waves ferromagnetic media and also in the description of two-dimensional shallow water waves (thereby generalizing the celebrated "Korteweg-de Vries equation"). A formal asymptotic analysis given in [34] connects the KP equation with a NLS of Davey-Stewartson type. Indeed the small dispersion limit of this model shares several similarities with the semi-classical limit for NLS. We expect to continue our studies of the KP model, aiming for establishing numerically different qualitative properties, in the nearby future.

**d) Semiclassical limits of NLS**
We consider the NLS with a "small parameter" $\epsilon$ that typically also enters as a scale of oscillations in the initial data $\psi_I^\epsilon$ :

$$i\epsilon\partial_t\psi^\epsilon = -\frac{\epsilon^2}{2}\Delta\psi^\epsilon + V^\epsilon(x,t)\psi^\epsilon \tag{9}$$

The "homogenization" limit of $\epsilon \to 0$ in this NLS corresponds to a "(semi)classical limit" of vanishing scaled Planck constant or to a "high wave number limit" in nonlinear optics, where such NLS is obtained as the paraxial approximation of the Helmholtz equation.
The physically interesting quantities like the "density" $n = |\psi^\epsilon|^2$ are quadratic in $\psi^\epsilon$. Since we are in the regime of weak limits (concentrations and oscillations), the calculation of such quadratic quantities does not commute with the limit, of course.

Wigner transform methods have proven to be a very good tool for analytical results for such "semiclassical limits" : a general theory for wide classes of linear problems was given in [21]. Also weakly nonlinear problems of Schrödinger-Poisson type could be successfully tackled e.g. [60] and [12] where the setting is in a crystal which is relevant for semiconductor modeling. Such kind of results have been used for theoretical analysis of numerical algorithms [51], however, the Wigner transforms have only limited interest for numerical simulations, where WKB methods and their generalizations have turned out to stay the preferable tool.
We recall the basic WKB ansatz :

$$\psi^\epsilon(x,t) = a(x,t)e^{iS(x,t)/\epsilon}\,,$$

The relation of Wigner transform methods to Multiphase WKB methods has been first studied by the proposers in [57], where the general linear case is discussed.

Further theoretical studies on WKB methods have been performed by the proposers for Schrödinger-Poisson systems e.g. in [20] and in [19] (where a periodic lattice potential is included).

The proponents have started numerical simulations of semiclassical limits for Schrödinger equations in a crystal using "multi branch" WKB methods (based on ideas of Y. Brenier [18]) : for the linear case in [27] and for the weakly nonlinear case of coupling to the Poisson equation [26].

These numerical methods and results shall be extended to more realistic situations and other applications of semiclassical NLS.

2.4. **ad (iv): quantum Boltzmann equations.** Using the Wigner function formalism, the Levinson equation

$$\partial_t f = \int_0^t \int_B [S(k,k',t-t')f(k',t') - S(k',k,t-t')f(k,t')]dk'\,dt'$$

has recently been derived as the weak coupling limit of a one electron and arbitrarily many phonons system [37], where the phonons represent a quantum description of oscillations of a semiconductor crystal. Here $f = f(k,t)$ is the electron distribution in dependence of the wave vector $k \in B$, where the (bounded) Brillouin zone $B \subset R^3$ is a basic cell of the dual of the semiconductor crystal lattice. The distribution $f$ is $B$-periodic. Explicit expressions for the scattering rate $S$ can be derived.

In a large time scale limit, the scattering operator of the Levinson equation converges to Fermi's Golden Rule and a first order correction term [45]. While implementations of Levinson's scattering operator, which is non-local in time, are extremely memory-consuming, the quantum correction term involves only time-derivatives of the Wigner function. The Levinson and closely related equations will be studied. Existence and uniqueness results for model problems will be derived, and qualitative properties such as equilibria and long time behavior will be investigated. The next aim will be the derivation of quantum scattering operators in the context of spatially inhomogeneous models for transport. Asymptotic methods will be used based on assumptions such as equilibrium for the phonon system and weak scattering. The aims are accurate, but still computable quantum scattering and transport models. The final goal is the incorporation of the new models in semiconductor simulation programs.

2.5. **ad (v): stochastic numerical methods for kinetic equations.** The seminal work [43] by T. Lyons and N. Victoir, which introduced the concept of cubature on Wiener space, stimulated recent efforts to improve numerical methods for stochastic differential equations and for the corresponding Fokker-Planck equations, i.e., convection-diffusion equations, often with degenerate diffusion (e.g. the current FWF project *Cubature on Wiener Space*, led by C. Schmeiser). The basic idea is to replace the Wiener process, i.e., the Brownian motion $B(t)$, which drive the Stratonovich differential equations

$$d\xi = V_0(\xi)dt + V_1(\xi) \circ dB\,,$$

by a finite probability space, i.e., a finite set of deterministic paths $\omega_1(t), \ldots, \omega_N(t)$ with probabilities $\lambda_1, \ldots, \lambda_N$, carefully chosen such that expectation values $E(f(\xi(T)))$ computed from the solution are approximated with a certain accuracy by $\sum_{i=1}^N f(y_i(T))\lambda_i$, where $y_i$ is the solution of the ODE

$$dy_i = V_0(y_i)dt + V_1(y_i)d\omega_i\,.$$

It is far from trivial and the subject of intensive investigations to design efficient numerical algorithms based on this idea. However, some very promising results have already been achieved for applications in Mathematical Finance [47].

We propose to extend the cubature idea to differential equations driven by Poissonian jump processes. Here the whole theory has to be developed from the beginning (although a first step has been taken recently in [22]). Since kinetic transport equations with scattering integrals can be seen as master equations for velocity jump processes, this may lead to new types of numerical approaches with the potential of improving standard Monte Carlo simulation methods. A connection to topic (iv) is possible if a probabilistic interpretation of the quantum corrections to the semiclassical transport model can be found.