Research highlights

Stochastic biochemical networks.

Elementary biochemical reactions in living cells are organized in networks to perform more complicated tasks. Theoretical and numerical study of these networks is complicated by mesoscopic character of many processes. Typically, the number of available molecules is so small that reactions must be considered as chains of discrete stochastic events. Numerical simulations of such stochastic processes are usually very challenging already for a relatively small number of chemical species.

We are interested in understanding how signals propagate through stochastic biochemical networks of various complexity. Specific questions include deriving (asymptotocally) exact results for coarse-graining biochemical kinetics in the context of dynamical signals (e.g., concentrations of various chemicals that change over time due to external influences and/or due to noise). The methods used involve WKB (mesoscopic molecular copy numbers) techniques, full counting statistics methods, and Doi-Peliti formalism. We are specifically interested in simple model reactions, like Michaelis-Menten (or particle transport), Hill cooperative reactions, protein-DNA binding, and others.

Berry phase in stochastic kinetics.

The analysis of time-scale separation of fast and slow variables in stochastic processes uncovers an unusual phenomenon, which can be theoretically considered as the Berry phase effect in purely classical stochastic dynamics. The Berry phase provides an elegant unifying quantitative theory for a plethora of effects in nonequilibrium statistics, such as the reversible ratchet effect and stochastic pump.

[1] N. A. Sinitsyn, and I. Nemenman, "*The Berry phase and the pump flux in stochastic chemical kinetics*", Europhys. Lett. 77, 58001 (2007)
[2] N. A. Sinitsyn, and I. Nemenman,

Anomalous Hall effect.

Despite its long (over 50 years) history, the theory of the Anomalous Hall Effect continues to be the subject of confusion and debates. Rigorous Hall current calculations by Green function techniques have been very involved and not physically transparent. Farraginous theoretical results have followed from the application of different methods to the same models.

We designed the semiclassical theory of the anomalous Hall effect which goal was to derive all contributions to the Hall conductivity via a strongly simplified approach, based only on the semiclassical Boltzmann equation and wave packet equations of motion. This approach operates only with gauge invariant values and thus all expressions acquire a clear physical interpretation. The connection of quantum mechanical description of scattering and transport processes with purely classical concepts is achieved via a set of specially derived rules, that are akin and include the Fermi's golden rule of quantum mechanics. The semiclassical theory is rigorous, i.e. in the diffusive regime it leads to the same quantitative predictions as the formally exact approach based on the Kubo-formula

[1] N. A. Sinitsyn, A.H. MacDonald, T. Jungwirh, V. K. Dugaev and J. Sinova, “*Anomalous Hall effect in 2D Dirac band: link between Kubo-Streda formula and semiclassical Boltzmann equation approach*”, Phys. Rev. B **75**, 045315 (2007)
[2] N. Sinitsyn, Q. Niu, J. Sinova, K. Nomura, Phys. Rev. B **72**, 045346 (2005)

Spin Hall effect.

In 2004 the intrinsic spin Hall effect was proposed as a novel spintronic effect. The intrinsic spin Hall effect is analogous to the intrinsic anomalous Hall effect in ferromagnets [*"Infrared magneto-optical properties of (III,Mn)V ferromagetic semiconductors"*, Phys. Rev. B 67, 235203 (2003)] but does not require to work with ferromagnetic materials. By manipulating the electron's spin degreee of freedom, we would have a richer *spintronic* device.

[1] Jairo Sinova, Dimitrie Culcer, Q. Niu, N. A. Sinitsyn, T. Jungwirth, A.H. MacDonald, *"Universal Intrinsic Spin-Hall Effect"*, Phys. Rev. Lett. 92, 126603 (2004)
[2] N. A. Sinitsyn, J. E. Hill, H. Min, J. Sinova, and A. H. MacDonald, “*Charge and Spin Hall Conductivity in Metallic Graphene*”, Phys. Rev. Lett. **97**, 106804, (2006)

Multistate Landau-Zener theory.

Simple exact results in non-stationary quantum mechanics are rare but very influential. Thus the quantum mechanical solution of a harmonic oscillator problem with time-dependent force strongly advanced the theory of decoherence. The Landau-Zener model is another widely used example of an exactly solvable explicitly time dependent system. Its central result is the Landau-Zener formula, which provides the probability of a transition between two states after time-dependent avoided crossing of their adiabatic energy levels.

Until recent time, generalizations of the Landau-Zener model to a higher number of states had been considered intractable analytically. We have achieved substantial progress in exact treatment of several classes of multistate Landau-Zener systems. Our results already found applications in physics of nanomagnets, Bose condensates and the theory of decoherence.

[1] B. E. Dobrescu, N. A. Sinitsyn, 2006 *J. Phys. B: At. Mol. Opt. Phys.* **39** 1253
[2] N. A. Sinitsyn, 2004 *J. Phys. A: Math. Gen.* **37** 10691

Landau-Zener transitions with decoherence.

Many applications of the Landau-Zener theory to externally driven nanoscopic systems require a rigorous account for decoherence. We derived the general formula for the Landau-Zener transition probability in the presence of a fast classical noise and explored effects of other types of noisy environment, such as the nuclear spin bath.

[1] V. L. Pokrovsky and N. A. Sinitsyn, "*Fast noise in the Landau-Zener theory*", Phys. Rev. B **67**, 045603, (2004)
[2] N.A. Sinitsyn and V. V. Dobrovitski, "*Nuclear spin bath effects in molecular nanomagnets: direct quantum mechanical simulations*", Phys. Rev. B **70**, 174449, (2004)