Master in Physics M2 2018-2019

Stage project proposal

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Project title: *Geometrical and Topological investigation of Phase Transitions*

Framework: One of the main topics in Statistical Mechanics concerns phase transitions phenomena. From the theoretical viewpoint, understanding their origin, and the way of classifying them, is of central interest.

Usually, phase transitions are associated with a spontaneous symmetry-breaking phenomenon: at low temperatures the accessible states of a system can lack some of the global symmetries of the Hamiltonian, so that the corresponding phase is the less symmetric one, whereas at higher temperatures the thermal fluctuations allow the access to a wider range of energy states having all the symmetries of the Hamiltonian. In the symmetry-breaking phenomena, the extra variable which characterizes the physical states of a system is the order parameter. The order parameter vanishes in the symmetric phase and is different from zero in the broken-symmetry phase. This is the essence of Landau's theory. If G_0 is the global symmetry group of the Hamiltonian, the order of a phase transition is determined by the index of the subgroup $G \subset G_0$ of the broken symmetry phase. The corresponding mechanism in quantum field theory is described by the Nambu–Goldstone's Theorem.

However, this is not an all-encompassing theory. In fact, many systems do not fit in this scheme and undergo a phase transition in the absence of a symmetry-breaking. This is the case of liquid–gas transitions, Kosterlitz–Thouless transitions, coulombian/confined regime transition for gauge theories on lattice, transitions in glasses and supercooled liquids, in general, transitions in amorphous and disordered systems, folding transitions in homopolymers and proteins, to quote remarkable examples. All these physical systems lack an order parameter.

Moreover, classical theories, as those of Yang–Lee and of Dobrushin–Lanford–Ruelle, require the $N \to \infty$ limit (thermodynamic limit) to mathematically describe a phase transition, but the study of transitional phenomena in finite N systems is particularly relevant in many other contemporary problems, for instance related with polymers thermodynamics and biophysics, with Bose–Einstein condensation, Dicke's superradiance in microlasers, nuclear physics, superconductive transitions in small metallic objects. The topological theory of phase transitions provides a natural framework to get rid of the thermodynamic limit dogma because clear topological signatures of phase transitions are found already at finite and small N in some submanifolds of both phase space and configuration space [1,2,3].

Aim of the stage: The work to be done during this stage will be both analytical and numerical. The focus will be on the investigation of phase transition phenomena occurring in the absence of symmetry-breaking, and thus in the absence of an order parameter. The model initially chosen will be the classical Heisenberg planar XY model in two spatial dimension which is known to undergo a Kosterlitz-Thouless phase transition. The study will proceed by numerically integrating the Hamilton equations of motion of this model and thus computing total geometrical quantities of the constant energy level sets in phase space, and of the equipotential level sets of configuration space. The relevant geometric quantities will be chosen so as to apply the Gauss-Bonnet-Hopf, the Chern-Lashof, and the Pinkall theorems of differential topology to the constant energy hypersurfaces in phase space. The ergodic invariant measure of Hamilton equations of motion is the microcanonical measure on these constant energy hypersurfaces thus allowing to apply the mentioned theorems through the numerical integration of the equations of motion of the model under investigation. Whereas, the computation of the required geometric quantities of the equipotential hypersurfaces of configuration space has to be performed along a Monte Carlo Markov chain given by the numerical solution of the stochastic differential equation

$$dR = P(R)\, dB + M_1 (R) n(R) dt$$

where R_t, $t \geq 0$, is a random sequence of points on $\Sigma_V \subset R^N$, $P(R) = I - n(R) \otimes n^T (R)$ is the orthogonal projection of a point R on the plane tangent to Σ_V at R, provided that $n \equiv \nabla V/\|\nabla V\|$ (normal at R); B is a Brownian motion in R^N and $M_1(R)$ is the mean curvature at R, that is, $M_1 = -\operatorname{div} n(R)/N$.

By numerically computing the Gauss–Kronecker curvature of the hypersurfaces under investigation, a topological invariant as the Euler–Poincaré characteristic can be obtained through the Gauss-Bonnet-Hopf theorem providing precious and direct information about the kind of topology changes, if any, at the transition point.

Beside the computation of the geometric quantities mentioned above, also the energy dependence of the largest Lyapunov exponent, computed by means of the simultaneous integration of the Hamiltonian dynamics and of the tangent dynamics, will provide indirect but reliable informations concerning non-trivial topological transition in configuration space at the Kosterlitz-Thouless phase transition point.

Some analytical computation – even approximate - of the Morse indexes will be also attempted on the basis of the exactly solvable XY model in one dimension and of the mean-field version of the same model.

References:

1) Marco Pettini, *Geometry and Topology in Hamiltonian Dynamics and Statistical Mechanics*, (Springer, New York, 2007). PDF file provided by the supervisor
2) M. Gori, R. Franzosi and M. Pettini, *Topological origin of phase transitions in the absence of critical points of the energy landscape*, J. Stat. Mech. 093204 (2018).
3) G. Pettini, M. Gori, R. Franzosi, C. Clementi and M. Pettini, *On the origin of phase transitions in the absence of symmetry-breaking*, Physica A516, 376 (2018).