# Lyapunov exponents at the liquid-vapor critical transition

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Fluids are a prototypical example of chaotic motion at molecular level. In fact, a fluid will generally have very many positive Lyapunov exponents (LEs) associated with the erratic evolution of the microscopic degrees of freedom (position and momenta) of its constituent molecules. Real fluids can be found in two different phases, vapor and liquid, which can also coexist in a certain region of the temperature-density $(T, \rho)$ phase diagram, bounded by the coexistence line. Above the coexistence line the fluid has uniform density, while below the coexistence curve we find two well separated phases of very different density. The coexistence curve has a maximum and terminates at the liquid-vapor critical point $(T_c, \rho_c)$.

All this is very well-known and understood from basic equilibrium statistical mechanics. However, there is not currently a full understanding of the mechanical instability in the molecular motion at this critical point nor at the coexistence line. For instance, we do not still know how to characterize the liquid-vapor transition or its coexistence in terms of the underlying microscopic dynamics for simple 3D fluids models. How do the LEs change at the transition? Can we establish a phase change in a fluid by looking only at microscopic dynamics? In other words, what are the fingerprints of a phase change in terms of LEs and Lyapunov vectors?

Here, we couple techniques from nonlinear dynamics and statistical physics to analyze the emergence of the phase of coexistence in the prototypical Lenard-Jones model of a 3D fluid. By means of numerical simulations we show that the largest LE exhibits a dramatic drop at the coexistence curve. Calculation of the inverse participation ratio shows that this LE drop is accompanied by a strong localization of the Lyapunov vector, marking a change in the dominant microscopic instability: from localized to spatially extended Lyapunov modes. We also show that the functional dependence of the LE with temperature (or density) allows to determine the spinodal curve that separates the phase coexistence region from the metastablility (supercooled vapor) region. All these results are new and pave the way to understand the liquid-vapor transition in purely dynamical terms.