Microscopic chaos and diffusion of single particles in periodic lattices

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Abstract

Modern theories of nonequilibrium statistical mechanics sometimes start from the assumption of *microscopic chaos* in the motion of atoms and molecules. Such a chaotic hypothesis models the fact that diffusion of single particles is generated by microscopic equations of motion which typically are highly nonlinear. In my talk I will first review the concepts of deterministic chaos and diffusion. I will then outline a theoretical approach which enables to understand diffusion on the basis of microscopic deterministic chaos [1]. Simple models ranging from deterministic versions of random walks on the line to molecular diffusion in periodic arrays of scatterers will be studied analytically and by computer simulations. Surprisingly, the diffusion coefficients of these models turn out to be highly irregular (fractal) functions of control parameters while simple random walk theory predicts monotononicity. This is due to correlated microscopic scattering events, which vary in a complicated way under parameter variation. I will argue that such phenomena should typically be seen in experiments on single particle diffusion in periodic lattices and in kicked rotor-like systems.

[1] R.Klages, Microscopic Chaos, Fractals and Transport in Nonequilibrium Statistical Mechanics (World Scientific, Singapore, 2007)