Negative cooperativity of transient characteristics of a system with fluctuating energy levels

O.L. Kapitanchuk and V.I. Teslenko

Bogolyubov Institute for Theoretical Physics, NAS of Ukraine,
14-b Metrologichna Str., Kyiv 03680, Ukraine

In the framework of an open quantum system coupled to a condensed medium and, thus, experienced relaxation transitions between different states and thermal fluctuations of level energies, a microscopic model of the process of irreversible binding between the ligand and the receptor molecule in solution is developed. Analytical expressions for the occupancies of intermediate (i.e., transient) states of a system averaged over an equilibrium Bose distribution of vibrational transitions in the medium and the stationary white-noise like distribution of random energy shifts in the system are derived. It is shown that in the presence of at least one irreversible kinetic stage, calculated dependence of the amplitude of transient occupancies on the ligand concentration essentially reveals a property of systems negative cooperativity. In several cases considered, such a property becomes most apparent in Hill coefficients which are generally reduced to some nonintegral values in comparison with particular integer numbers being an initial characteristic to the system. Also, it is found that this effect is influenced additionally both by the degree of system heterogeneity and by the intensity of fluctuations of the system energies. Moreover, it is observed that such phenomena are normally acting in a consensus providing for the most prominent evidence of negative cooperativity effect as in the mostly heterogeneous systems as well in those exhibiting the most high-intensive energy fluctuations.