Coarse-grained kinetic equations for quantum systems

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A nonequilibrium density matrix method is employed to derive a master equation for the averaged state populations of the open quantum systems. Averaged procedure is associated with action of the fast stochastic fields created either by external sources or fluctuations of interior structure groups of the condensed media. The averaging procedure allows one to reduce the stochastic master equation for a density matrix of the quantum system to the kinetic equation for the averaged state populations if only the characteristic time τ_{stoch} of fast stochastic processes is much less the characteristic time τ_{steady} of transition processes responsible for the establishment of steady state populations in the system. Thus, on the time scale $\Delta t \gg \tau_{stoch}$ the averaged master equation appears as the coarse-grained kinetic equation. If a quantum system consists of several subsystems, then, generally, a kinetic equation for state populations of the separate subsystem can appears as a nonlinear kinetic equation [1]. Linearization becomes possible if a quantum system interacts with quantum or classic systems supported in the equilibrium states. Special case of kinetic processes is considered for quantum systems where the kinetics is dictated by isoenergetic transitions. It is shown that for such type of systems, the thermodynamic fluctuations are able to cancel a temperature dependence for the rate constants [2]. Another example is the description of an electron transfer from one macroscopic system to another macroscopic system through a small quantum system. It has been shown that a formation of the particle flow through a quantum system is dictated by the contact charge hopping processes between the quantum system and each macroscopic system as well as a direct electron tunneling mediated by a quantum system. In the second case, the states of quantum systems participate in the transfer process as virtual states [3,4].

[1] E. G. Petrov, Ukr. J. Phys. **55**, 121, 2010.

[2] E. G. Petrov and V. I. Teslenko, Chem. Phys. **375**, 243, 2010.

[3] E. G. Petrov, Ukr. J. Phys. **56**, 721, 2011.

[4] E. G. Petrov, Ye. V. Shevchenko, V. May and P. Hänggi, J. Chem. Phys. **134**, 204701, 2011.