

Generalized diffusion coefficients in multicomponent fluids

I. Mryglod, V. Kuporov and O. Prytula

*Institute for Condensed Matter Physics of the National Academy of Sciences of Ukraine, 1 Svientsitskii Str., 79011 Lviv, Ukraine,
E-mail: slw@icmp.lviv.ua*

The problem of definition for diffusion coefficients in the multicomponent systems as well as their representation in different reference frames is considered. We perform analytic study of mutual diffusion coefficients within the frames of generalized modes approach. Using the rigorous mathematical formalism the matrix of generalized diffusion coefficients depended on the wave vector and time are obtained as product of the generalized kinetic coefficients matrix and the matrix of static structure factors. In the hydrodynamic limit corresponding Green-Kubo formulas for diffusion coefficients are derived.

With help of simple matrix transformations it is shown that all mutual diffusion coefficients can be reduced to $\nu(\nu-1)/2$ independent dynamical quantities expressed via the corresponding correlation times. Here ν is the number of species in the mixture. The structure of transformation matrixes are found. This allows us to study in detail the transformations between different reference frames and to derive the correct expression for mutual diffusion coefficients.

In order to give an example our approach is used for the study of conductivity properties in a multicomponent charged particles system. In particular, we derived so-called "universal gold rule" for the ratio of partial conductivities for the model of molten salts.