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Transport properties for an electroneutral Yukawa-type fluid in the MSA

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Abstract

In the framework of a linear response theory, in which Onsager's continuity equations are combined with the Mean Spherical Approximation (MSA) from the theory of correlation functions in equilibrium, and using a Green's function formalism, we consider the transport properties of electrolytes. The interaction between the ions in the electrolyte is represented by an intermolecular Yukawa potential which satisfies the electroneutrality condition. The model contains an adjustable parameter z which takes into account the effects of the solvent. Transport processes in an ionic solution are determined by two dominant forces: the relaxation and the electrophoretic forces; their contributions to the transport properties are calculated using the Fuoss-Onsager theory. We find the conductivity and the self-diffusion coefficient for a family of electrolytes using the linear response theory. The predictions of our model can be adjusted by means of the parameter z . The electrophoretic effect, due to the hydrodynamic interaction between the ions, is calculated using the Rotne-Prager tensor. Our theoretical results are in good agreement with experimental data for electrolytes 1-1, even for high concentrations. We applied this theory also to two unsymmetrical electrolytes, namely the aqueous solutions of MgCl_2 and CaCl_2 , with results in good accord with experimental data.

Key-words:

Electroneutral Yukawa fluid, transport properties, electrophoretic effect, hydrodynamic interaction, Fuoss-Onsager theory.

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1 Introduction

Understanding and predicting the behavior of phenomena occurring in plasmas and electrolytical systems is a very interesting area of research, not only in physics and

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