

Global isomorphism between Buckingham and Yukawa fluids and Lattice gas

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Global isomorphism is based on the idea of similarity of behavior of a simple fluid and lattice gas in entire liquid-vapor coexistence region. This “similarity” can be approximated by the projective map between the thermodynamic states of these systems.

$$n = n_* \frac{x}{1 + zt}, \quad T = T_* \frac{zt}{1 + zt}, \quad (1)$$

where (x, t) - describe state of lattice model. (T_*, n_*) - so called the parameters of the Zeno-element and represent the “limit” states of fluid system. We discuss their difference from commonly used Boyle temperature and density respectively.

We show how global isomorphism approach can be modified for the cases of the Buckingham:

$$\Phi_B(x; a) = \begin{cases} \infty, & x \leq r_0/r_m, \\ \frac{\varepsilon}{1-6/a} \left(\frac{6}{a} \exp(a(1-x)) - \frac{C}{x^6} \right), & x > r_0/r_m, \end{cases} \quad (2)$$

and the hard-core attractive Yukawa:

$$\Phi_Y(r; \gamma) = \varepsilon \frac{\exp(-\gamma(r-\sigma))}{r} \quad r > \sigma \quad (3)$$

potentials using the idea of homogeneity transformation within the potentials of Mie-class. This modification allows to describe the critical parameters for Buckingham potential and check the agreement with numerical data. We check a number of linear relations which are simple consequences of (1), among them the relation of the critical point line:

$$\frac{2n_c}{n_*} + \frac{T_c}{T_*} = 1 \quad (4)$$

Violation of this condition makes it possible to predict the disappearance of the liquid binodal branch, when the potential (3) becomes too short-ranged.