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A. Maslechko, K. Glavatskiy, V.L. Kulinskii

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Surface tension of molecular liquids: Lattice gas approach

A. Maslechko^a, K. Glavatskiy^b, V.L. Kulinskii^{c,*}

^a*Department of Chemistry, Norwegian University of Science and Technology, Høgskoleringen 5, N-7491 Trondheim, Norway*

^b*School of Chemical Engineering, The University of Queensland, Australia*

^c*Department of Theoretical Physics, Odessa National University, Dvoryanskaya 2, 65082 Odessa, Ukraine*

Abstract

The approach of global isomorphism between the fluid and the Ising model is applied to obtain an expression for the surface tension of the Lennard-Jones fluid on the basis of the information about the Ising model. This is done in a broad interval of temperatures along the phase coexistence, and is valid both in a 2D and a 3D. The relation between the critical amplitudes of the surface tension of the fluid and the Ising model is derived in the vicinity of the critical point. The obtained theoretical estimates agree well with the literature results for the surface tension. The methodology is demonstrated for the 2D LJ fluid on the basis of the exact solution of the 2D Ising model and is tested for the 3D LJ fluid. As a result, an expression for the surface tension without any fitting parameter is derived.

Keywords: Surface tension, lattice gas, global isomorphism

PACS: 64.70, 68.40

1. Introduction

The surface tension is one of the most vivid properties of a fluid. Theoretical descriptions, which employ methods of homogeneous statistical mechanics, are challenging to use due to lack of symmetry at the phase boundary,

*Corresponding author

Email addresses: anastasiia.maslechko@ntnu.no (A. Maslechko),
(kulinskij@onu.edu.ua) (V.L. Kulinskii)

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