### Accepted Manuscript

### Research paper

Transport coefficients of normal liquid helium-4 calculated by path integral centroid molecular dynamics simulation

Haruna Imaoka, Kenichi Kinugawa

PII:	S0009-2614(17)30046-5
DOI:	http://dx.doi.org/10.1016/j.cplett.2017.01.034
Reference:	CPLETT 34472
To appear in:	Chemical Physics Letters
Received Date:	30 November 2016
Revised Date:	10 January 2017
Accepted Date:	15 January 2017



Please cite this article as: H. Imaoka, K. Kinugawa, Transport coefficients of normal liquid helium-4 calculated by path integral centroid molecular dynamics simulation, *Chemical Physics Letters* (2017), doi: http://dx.doi.org/10.1016/j.cplett.2017.01.034

This is a PDF file of an unedited manuscript that has been accepted for publication. As a service to our customers we are providing this early version of the manuscript. The manuscript will undergo copyediting, typesetting, and review of the resulting proof before it is published in its final form. Please note that during the production process errors may be discovered which could affect the content, and all legal disclaimers that apply to the journal pertain.

## ACCEPTED MANUSCRIPT

### Revised manuscript to Chemical Physics Letters

## Transport coefficients of normal liquid helium-4 calculated by path integral centroid molecular dynamics simulation

Haruna Imaoka<sup>\*</sup> and Kenichi Kinugawa<sup>\*\*</sup>

Division of Chemistry, Graduate School of Humanities and Sciences, Nara Women's University, Nara, 630-8506, Japan

### Abstract

Thermal conductivity, shear viscosity, and bulk viscosity of normal liquid <sup>4</sup>He at 1.7-4.0 K are calculated using path integral centroid molecular dynamics (CMD) simulations. The calculated thermal conductivity and shear viscosity above lambda transition temperature are on the same order of magnitude as experimental values, while the agreement of shear viscosity is better. Above 2.3 K the CMD well reproduces the temperature dependences of isochoric shear viscosity and of the time integral of the energy current and off-diagonal stress tensor correlation functions. The calculated bulk viscosity, not known in experiments, is several times larger than shear viscosity.

Keywords: computer simulation, liquid helium-4, thermal conductivity, shear viscosity, bulk viscosity, path integral centroid molecular dynamics

#### 1. Introduction

For many decades liquid <sup>4</sup>He has attracted extensive attention especially regarding the superfluid state into which it changes the phase at the lambda transition temperature  $T_{\lambda}$ , where  $T_{\lambda} = 2.17$  K at saturated vapor pressure (SVP) [1-3]. Observed superfluidity such as the divergence of thermal conductivity and the remarkable decrease of viscosity is caused by large quantum dispersion of atoms, weakness in interatomic interaction, and atomic exchange effect due to Bose statistics. Superfluidity is explained in term of, for instance, Landau's *two-fluid* theory [4] where liquid <sup>4</sup>He below  $T_{\lambda}$  is considered as a mixture of two components, i.e. normal fluid with nonzero viscosity and superfluid with zero viscosity, and the fraction of the superfluid component increases from zero at  $T_{\lambda}$  with decreasing temperature [1].

24

<sup>\*</sup> Present address: NEC Solution Innovators, Ltd., Shiromi, Chuo-ku, Osaka 540-8551, Japan.

<sup>\*\*</sup> Corresponding author. E-mail address: kinugawa@cc.nara-wu.ac.jp.

Download English Version:

# https://daneshyari.com/en/article/5378154

Download Persian Version:

https://daneshyari.com/article/5378154

Daneshyari.com