Physica A 423 (2015) 27–32

Contents lists available at ScienceDirect

Physica A

journal homepage: www.elsevier.com/locate/physa

Comment on analysis of transport properties determined by Langevin dynamics using Green–Kubo formulae

Stefan Heinz *

University of Wyoming, Department of Mathematics, 1000 East University Avenue, Laramie, WY 82071, USA

HIGHLIGHTS

- Molecular dynamics simulations based on Langevin models are considered.
- A correction is presented for the Green–Kubo Prandtl number derived by Zhang et al.
- The relationship between Green–Kubo and Boltzmann equation Prandtl numbers is analytically explained.

ARTICLE INFO

Article history:
Received 2 September 2014
Received in revised form 11 December 2014
Available online 31 December 2014

Keywords:
Langevin dynamics
Boltzmann equation
Green–Kubo formulae
Transport coefficients

ABSTRACT

The development of Langevin models for molecular dynamics represents a promising approach to deal with the cost issue of Boltzmann equation solutions. A recent paper of Zhang et al. suggested to study the Prandtl number variability of such molecular Langevin models under equilibrium conditions. This paper comments on several questions related to the approach of Zhang et al. First, a correction is presented for the Green–Kubo minimum Prandtl number derived by Zhang et al. Second, the relationship between the Green–Kubo Prandtl number and a Prandtl number defined in the Boltzmann equation sense is analytically explained. Third, based on this relationship it is shown that the consideration of a Prandtl number defined in the Boltzmann equation sense represents a more appropriate approach to address the question considered.

1. Introduction

A paper recently published by Zhang et al. [1] investigates a Langevin acceleration model, which was proposed by Heinz [2] as a molecular model for fluid flow. The purpose of the paper by Zhang et al. is the exact calculation of fluid flow transport properties as determined by Heinz's acceleration model and a related velocity model for molecular motion. A problem of Langevin molecular models is the correct treatment of heat transport, which is reflected by incorrect Prandtl numbers predicted by some models [1–5]. Thus, a specific question addressed by Zhang et al. [1] is whether or not Heinz's acceleration model is capable of providing a correct Prandtl number.

The purpose of this paper is to comment on the paper of Zhang et al. [1]. Results previously obtained by Heinz [2] and Zhang et al. [1], which are relevant to the following discussion, will be described in Section 2. Section 3 deals with comments on the results of Zhang et al. [1]. Conclusions will be presented in Section 4.

* Tel.: +1 307 766 4203; fax: +1 307 766 6838.
E-mail address: heinz@uwyo.edu.

http://dx.doi.org/10.1016/j.physa.2014.12.022
0378-4371/

2. Previously obtained results

Results presented in Ref. [2] will be summarized in the next two paragraphs. Heinz suggested the following acceleration model as a molecular model of monatomic fluids which do not have internal degrees of freedom (rotational or vibrational energy),

$$\frac{\mathrm{d}x_i^*}{\mathrm{d}t} = V_i^*, \tag{1a}$$

$$\frac{\mathrm{d}V_i^*}{\mathrm{d}t} = A_i^*, \tag{1b}$$

$$\frac{\mathrm{d}A_i^*}{\mathrm{d}t} = \frac{1}{\tau_a}\left\{-A_i^* - \frac{1}{\tau_m}\left(V_i^* - U_i\right) + \sqrt{\frac{4e}{3\tau_m}}\frac{\mathrm{d}W_i}{\mathrm{d}t}\right\}. \tag{1c}$$

The state of each molecule is completely described by its Lagrangian position x_i^*, velocity V_i^*, and acceleration A_i^*. Here, t is time, and $i = 1, 3$ refers to the space coordinate considered. The fluid velocity U_i, specific kinetic energy e, and characteristic time scales for molecular acceleration and velocity correlations, τ_a and τ_m, respectively, may depend on position and time. $\mathrm{d}W_i/\mathrm{d}t$ refers to a normally distributed process with vanishing means and uncorrelated values at different times,

$$\left\langle \frac{\mathrm{d}W_i}{\mathrm{d}t} \right\rangle = 0, \qquad \left\langle \frac{\mathrm{d}W_i}{\mathrm{d}t}\,(t)\,\frac{\mathrm{d}W_j}{\mathrm{d}t'}\left(t'\right)\right\rangle = \delta_{ij}\delta(t-t'). \tag{2}$$

Here, δ_{ij} is the Kronecker delta and $\delta(t-t')$ is the delta function. For simplicity, an external force (which may be caused, e.g., by gravity) is not considered. In the limit $\tau_a \to 0$, the acceleration model (1) turns into a velocity model,

$$\frac{\mathrm{d}x_i^*}{\mathrm{d}t} = V_i^*, \tag{3a}$$

$$\frac{\mathrm{d}V_i^*}{\mathrm{d}t} = -\frac{1}{\tau_m}\left(V_i^* - U_i\right) + \sqrt{\frac{4e}{3\tau_m}}\frac{\mathrm{d}W_i}{\mathrm{d}t}. \tag{3b}$$

The acceleration model can be used to derive the basic equations of fluid dynamics. The latter equations require closures for the stress tensor p_{ij} and heat flux q_k, which are defined by [6]

$$p_{ij} = \rho\,\overline{v_i v_j}, \qquad q_k = \frac{1}{2}\rho\,\overline{v_k v_n v_n}. \tag{4}$$

Here, $\overline{v_i v_j}$ and $\overline{v_k v_n v_n}$ refer to variances and third order moments of molecular velocities, respectively. In the lowest order of approximation, the acceleration model provides the expressions

$$p_{ij} = \frac{2}{3}\rho e\,\delta_{ij} - 2\,\mu\,S_{ij}^d, \qquad q_k = -\frac{\rho\gamma\nu}{\mathrm{Pr}}\frac{\partial e}{\partial x_k}. \tag{5}$$

The viscosity is given by $\mu = \rho\,\nu$, ρ refers to the fluid mass density, S_{ij}^d is the deviatoric rate-of-strain tensor, and the kinematic viscosity ν is given by

$$\nu = \frac{\tau_m e}{3}\left(1 + \frac{\tau_a}{\tau_m}\right). \tag{6}$$

In the heat flux expression we have $\gamma = 5/3$, and the Prandtl number Pr is given by

$$\mathrm{Pr} = \frac{3}{2}\left(1 + \frac{\tau_a}{\tau_m}\right)\left(1 + 0.5\,\frac{\tau_a}{\tau_m}\right)\left(1 + (2.5+\kappa)\,\frac{\tau_a}{\tau_m}\right)^{-1}. \tag{7}$$

It should be noted that $\mathrm{Pr} = \gamma\,N_{Pr}$. The symbol N_{Pr} was used in Ref. [2] to refer to the Prandtl number, as is some times done in regard to equations for turbulent flows [7]. In the latter expression we have $\kappa = 1 - (e/\tau_a\tau_m)\partial(\tau_a\tau_m)/\partial e$. The minimum Prandtl number $\mathrm{Pr}_{\min}$ is found at $(\tau_a/\tau_m)_{\min}$. The latter two minimum values are given by

$$\frac{\tau_a^{\min}}{\tau_m^{\min}} = \frac{\sqrt{2(\kappa+7/4)^2 - 1/8} - 1}{\kappa + 5/2}, \tag{8a}$$

$$\mathrm{Pr}_{\min} = \frac{3}{2}\left(1 + \frac{\tau_a^{\min}}{\tau_m^{\min}}\right)\left(1 + 0.5\,\frac{\tau_a^{\min}}{\tau_m^{\min}}\right)\left(1 + (2.5+\kappa)\,\frac{\tau_a^{\min}}{\tau_m^{\min}}\right)^{-1}. \tag{8b}$$

In particular, for $\kappa = 3.2467$ we find $\mathrm{Pr}_{\min} = 2/3$, the correct Prandtl number for a monatomic gas.