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Modeling of transport phenomena in gases based on quantum scattering

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HIGHLIGHTS

- A quantum interaction is implemented into direct simulation Monte Carlo method.
- *Ab initio* potential of interatomic interaction is applied.
- Two canonical problems of fluid mechanics are solved by the proposed method.
- The quantum scattering influence is significant in a wide range of the temperature.

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ABSTRACT

A quantum interatomic scattering is implemented in the direct simulation Monte Carlo (DSMC) method applied to transport phenomena in rarefied gases. In contrast to the traditional DSMC method based on the classical scattering, the proposed implementation allows us to model flows of gases over the whole temperature range beginning from 1 K up any high temperature when no ionization happens. To illustrate the new numerical approach, two helium isotopes ^{3}He and ^{4}He were considered in two canonical problems, namely, heat transfer between two planar surfaces and planar Couette flow. To solve these problems, the *ab initio* potential for helium is used, but the proposed technique can be used with any intermolecular potential. The problems were solved over the temperature range from 1 K to 3000 K and for two values of the rarefaction parameter $\delta = 1$ and 10. The former corresponds to the transitional regime and the latter describes the temperature jump and velocity slip regime. No influence of the quantum effects was detected within the numerical error of 0.1% for the temperature 300 K and higher. However, the quantum approach requires less computational effort than the classical one in this temperature range. For temperatures lower than 300 K, the influence of the quantum effects exceed the numerical error and reaches 67% at the temperature of 1 K. Numerical data provided in Supplemental Material can be used to model any kind of helium flow at any temperature.

1. Introduction

The direct simulation Monte Carlo (DSMC) method [1] used to calculate rarefied gas flows consists of decoupling of the free motion of gaseous molecules from collisions between them. The second stage requires a physical intermolecular potential in order to obtain reliable results. Recently, a procedure to implement any potential into the DSMC method was proposed in our previous paper [2] using the phenomenological Lennard-Jones potential as an example. In contrast

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to phenomenological models, *ab initio* (AI) potentials are free from any adjustable parameter usually extracted from experimental data. Nowadays, such potentials practically for all noble gases and their mixtures are available in the open literature, see e.g. [3–10]. Thus, the DSMC method based on AI potential [11] also becomes free from such adjustable parameters. The idea of the procedure to implement any potential into the DSMC is to generate look up tables of the deflection angle depending on the relative velocity of interacting particles and their impact parameter. The method was used to study the influence of the interatomic potential on various phenomena in rarefied gases [12–16] considering the intermolecular interaction based on the classical mechanics, that is justified at high temperatures for heavy gases. However, the quantum effects in intermolecular interactions is not negligible for light gases, e.g. helium, hydrogen, tritium, especially at moderately low temperatures [17–21]. It can be important to model helium, hydrogen and tritium flows in many technological fields such as cryogenic pumps [22,23], cryogenic systems used in the huge fusion reactor ITER [24,25], monochromatic beams of helium [26,27], helium microscope [28,29], acoustic thermometry at a low temperature [30,31], experimental set-up to measure the neutrino mass [32,33], etc. In spite of the high practical interest to model gases at low temperatures, the quantum scattering has not been implemented yet in the DSMC method.

The aim of the present paper is to propose a new technique to implement the quantum scattering into the DSMC method using any potential and to show the influence of quantum effects on transport phenomena in rarefied gases. For this purpose, a procedure of generation of deflection angle matrix based on quantum scattering is elaborated and a couple of classical problems of fluid mechanics is solved to evaluate the influence of quantum effects. A temperature range where the classical approach fails and the quantum theory becomes an unique alternative to simulate the transport phenomena in rarefied gases will be pointed out. It will be also shown that even at a high temperature when the classical approach works, the quantum approach reduces computational effort that makes it preferable for the whole range of the temperature. It should be emphasized that we are interested in quantum effects only in interatomic iterations. Other effects, like high densities at low temperatures when the interatomic distance is comparable to the de Broglie wavelength, are not considered here.

2. Numerical method

The DSMC method consists of a decoupling the free-motion of molecules from intermolecular collisions during each time steps Δt. Here, the free-motion of particles is considered to be classical that is valid under the condition [34,35]

$$\frac{nh^3}{(2\pi mk_{\mathrm{B}}T)^{3/2}} \ll 1, \tag{1}$$

where n is the gas number density, h is the Planck constant, m is the atomic mass of the gas, k_{B} is the Boltzmann constant and T is the gas temperature. This condition is well satisfied at the atmospheric pressure and at any temperature above the boiling point of both ^{3}He and ^{4}He that are 3.2 K and 4.2 K, respectively. For a temperature below the boiling point, the gas pressure must be low enough to keep helium in the gaseous phase and to meet the condition (1).

In the present paper, the quantum scattering is implemented in the stage of the intermolecular interactions. According to the no-time-counter version of the DSMC method [1], the number of pairs to be tested for collisions during a time step Δt in a cell of volume V_c reads

$$N_{\mathrm{coll}} = \frac{1}{2}N_p(N_p - 1)F_N(\sigma_{\mathrm{T}}g)_{\max}\frac{\Delta t}{V_c}, \tag{2}$$

where N_p is the number of particles in the cell, F_N is the number of real particles represented by one model particle, g is the relative speed of two interacting particles, σ_{T} is the total cross section (TCS) of particles which is a function of g according to the quantum theory of scattering, the quantity $(\sigma_{\mathrm{T}}g)_{\max}$ represents a maximum value of the product $\sigma_{\mathrm{T}}g$ in each specific cell. Then, N_{coll} pairs within the cell are chosen randomly. If a selected pair of particles satisfies the condition

$$\sigma_{\mathrm{T}}g/(\sigma_{\mathrm{T}}g)_{\max} > R_f, \tag{3}$$

the post-collision velocities are calculated; otherwise, the pre-collision velocities are kept. Here, R_f is a random fraction varying uniformly from 0 to 1. The relation of the post-collision velocities to pre-collision ones contains the deflection angle χ and impact angle ε, see Eqs. (8.32)–(8.35) from Ref. [36]. The angle ε is chosen randomly from the interval $[0, 2\pi]$, while the deflection angle χ should be calculated using the differential cross section (DCS) $\sigma(g, \chi)$ determined by the relative speed g. In contrast to the classical scattering used in the previous works [2,11–16], here the DCS is needed not only to calculate the post-collision velocity, but even to test a pair before to accept or to reject it.

Exact calculations of the DCS in the frame of quantum theory is a hard task and it is completely infeasible to do such calculations for each tested pair. To avoid all this job, look-up tables of the deflection angle χ generated once for some specific gas can be used for any flows of this gas. The authors of Ref. [37] also proposed to store the incomplete cross section and then they simulated a spatially homogeneous relaxation of helium in several background gases. However, they used an equally spaced mesh of the deflection angle that requires a rather long procedure to generate this angle for each binary collision. To reduce this effort significantly in the present work, the matrix of the deflection angles is generated by such a way that all its elements for some specific speed g are equally probable and can be chosen just randomly.