An Interlaced System for Rigid Rotors

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Abstract. The previously developed interlaced system [1] which can be used for problems where the cell Knudsen number may vary as $0 < Kn < \infty$ has been extended to include a further set of energy levels related to the internal energy of a rigid rotor. The evolution of a distribution function $f(r, c, e_i, t)$ is described by kinetic equations which are modified in such a way that molecular encounters with translational–rotational energy transfer are described using a transition probability $P_{ij}^{\alpha}(g)$, with $g$ as translational speed, and a molecular diameter $\sigma(g)$. The number of dimensions is reduced by replacing in the rhs—gain term of the kinetic equations the translational parts of the distribution functions by their Maxwells. Some preliminary numerical experiments were performed for the homogeneous case.

The Model of Molecular Interaction

Extending previous work [2,3], on the basis of results from MD calculations, we introduce a model for the molecular diameter

$$\dot{\sigma} = \sigma_{300} \frac{300}{T_{ref}} [1.016]$$

with $\sigma_{300} = 1.38\sigma_0$. Here $T_{ref}$ is to be understood as a “temperature” related to the translational kinetic energy of the interacting molecules.

After the separation of the cross section in the transition process, it is now necessary to develop a model for the transition averaged over $0 \leq b \leq \dot{\sigma}(g)$. With the use of MD calculations for large fields of the parameters $T_0$ (as a measure for the translational energy $e_{tr}$ or $g$), $J_1 = i$, and $J_2 = k$, we may model the transition probability as follows

$$P_{ij}^{\alpha} = P_0 \left\{ \alpha_0 \exp[-\Delta_1] + \frac{1}{\alpha_0} \exp[-\Delta_2] \right\},$$

where $\Delta_1, \Delta_2$ are combinations of energy differences, $\alpha_0$ is an adiabatic coefficient, and $P_0$ is a normalizing constant. A typical example for $T_0 = 100T_{ref}$, where $T_{ref} = \frac{Bhc}{k}$, $J_{1,2} = 10$ is given in Fig. 1(left); in Fig. 1(right) the model distribution is ,Eq. 2, presented. Note the exponential decay around the point $(i, k)$, the cutoff for $e_{tr} + e_{rj} + e_{rl} > e_{tot} = e_{tr0} + e_{rl} + e_{rk}$, and a preference of transition in the plains $i, k = \text{const.}$

The Kinetic Equation Model

We introduce a distribution function

$$f_{i}drdc = f(r, c, e_{ri}, t)drdc,$$

with a Maxwellian in the limit of equilibrium
FIGURE 1. Transition probability $P_{ij}^{kl}$ for $T_0 = 100T, g = 1$, and $j_1 = j_2 = 10$ Left: MD calculations; sample: 600,000 runs. Right: Model corresponding to Eq. 2.

$$f_{i,M} = \frac{n}{2\pi kT/m}^{3/2} \exp \left[-\frac{(c-u)^2}{2kT/m}\right] \frac{(2i+1)}{Q_r} \exp \left[-\frac{e_{rij}}{kT}\right].$$

Here $Q_r = \sum_{j=0}^{\infty} (2J+1) \exp[-J(J+1)T_r/T]$ is the state sum. Summation over all $i$ provides

$$f = \sum_i f_i.$$  (5)

The evolution of $f_i$ is governed by a Boltzmann kinetic equation of the kind

$$Df_i = R_i,$$  (6)

where $D = \partial/\partial t + c \cdot \nabla$ and

$$R_i = R(\mathbf{r}, c, e_{ri} ; t) = G_i - f_i \nu_i,$$  (7)

with

$$G_i = \sum_{jkl} \int f_j f_{ij} P_{ij}^{kl} g' \; db' \; d\varepsilon' \; dc'_1, \quad \nu_i = \sum_{jkl} \int f_{i,k} P_{ij}^{kl} g \; db \; d\varepsilon \; dc_1.$$  (8)

The relation of detailed balance is used to replace $P_{ij}^{kl}$. Thus, with the weight $w_{ij}^{kl}$

$$R_i = \sum_{jkl} \int [f_j f'_{i,j} w_{ij}^{kl} - f_i f_{i,k}] P_{ij}^{kl} g \; db \; d\varepsilon \; dc_1.$$  (9)

In the loss term the summation and the integration over $(b, \varepsilon)$ can be performed for this model

$$\nu_i = \pi \int \sum_k f_{1,k} \sum_{j,l} P_{ij}^{kl} g \; d\varepsilon \; dc_1.$$  (10)

With the definition of Eq. 5 we obtain

$$\nu_i = \pi \int f_{1} g \; d\varepsilon \; dc_1.$$  (11)

The term for the gain rate $G_i$ is of such a high dimension that it must be simplified for any practical application. With the property in mind that, in the limit, the gain function $f_g = G/\nu$ will approach a Maxwellian, we try the ansatz
\[ f_i = f_i^{tr}(c)\zeta_i, \]  

where \( \zeta_i = n_i/n \), and replace \( f_i^{tr} \) by \( f_i^{tr}_M \). Then the integrand has the form

\[ \exp \left[ -\frac{c_i^2 + c_i^2}{2kT/m} \right] \zeta_i \zeta_\jmath \phi_i^{kl} P_i^{kl}(g) g\sigma^2(g). \]

(13)

Now, using energy conservation, we replace \([c_i^2 + c_i^2]\) and obtain

\[ G_i = \pi f_{i,M} \sum_{jkl} f_{k,M} \left( \frac{\zeta_j}{\zeta_{j,eq}} \right) \left( \frac{\zeta_\jmath}{\zeta_{\jmath,eq}} \right) P_i^{kl}(g) g\sigma^2(g) dc_1. \]

(14)

We define

\[ \nu_i^+ = G_i/f_{i,M}. \]

(15)

After transformation from \( G_i \) to \( g \) the integral can be reduced to one dimension. Using the non-dimensional forms \( \xi^2 = C^2/(2kT/m) \) and \( \bar{g}^2 = g^2/(2kT/m) \) we obtain

\[ \nu_i^+ = 4n\sqrt{2\pi kT/m} \exp[-\xi^2] I_1, \]

(16)

with

\[ I_1 = \int_0^\infty \sum_{jkl} \zeta_j eq \zeta_\jmath eq \bar{P}_i^{kl}(\bar{g}) \left( \frac{\sigma(\bar{g})}{\sigma_0} \right)^2 \frac{\sinh 2\xi \bar{g}}{2\xi \bar{g}} \exp[-\bar{g}^2] \bar{g} \, d\bar{g}. \]

(17)

or, using the density \( n_0 \), the speed \( a_0 = \sqrt{\gamma_0 kT_0/m} \), and a length \( L_0 \) as reference quantities to non-dimensionalize, and with a Kundschen number \( K n_0 = [L_0 \pi (2n_0 \sigma_0^2)]^{-1} \), we have

\[ \nu_i^+ = \frac{2}{\sqrt{\pi} \gamma_0 K n_0} n\sqrt{T} \exp[-\xi^2] I_1. \]

(18)

When replacing the actual distribution function \( f_1 \) by \( f_{1,M} \) in the loss rate \( \nu_i \) we obtain

\[ \nu_M = \frac{2}{\sqrt{\pi} \gamma_0 K n_0} n\sqrt{T} \exp[-\xi^2] \int_0^\infty \left( \frac{\sigma(\bar{g})}{\sigma_0} \right)^2 \exp[-\bar{g}^2] \bar{g} \, d\bar{g}. \]

(19)

We introduce a gain function

\[ f_{i,g} = \nu_i^+ f_{i,M}/\nu_M. \]

(20)

Then the kinetic equation, as it shall be used in the following path integral, reduces to

\[ D f_i = \nu_M (f_{i,g} - f_i). \]

(21)

**Equation of Transfer (Upper Level System)**

Starting again from the basic kinetic equation, Eq. 6, multiplying it with the moments \( \psi = [m, mc, \frac{m}{2} c^2 + \sum_i c_{n_i} \] summing over all levels \( i \), and integrating over \( c \) provides the equation of transfer (the first five moment equations) for which the rhs vanishes

\[ \frac{\partial}{\partial t} Q_i + \nabla F_i = 0. \]

(22)

Here the moments can be written as
\[ Q_i = \left[ \rho, \rho u, \rho \left( \frac{3k}{2m} T + \frac{e_r}{m} \right) + \frac{p}{2} u^2 \right], \tag{23} \]

with the definition \( e_r = \sum_{i=0}^{j_{max}} e_{ri} \). The fluxes

\[ F_i = \sum_j \int \psi_i \psi_j \, dc \tag{24} \]

will, inside the interlaced system, not be expressed by terms consisting of products of lower moments and terms of higher moments like the shear tensor \( \sigma_{ij} \) and the heat flux \( q_i \), both related to the center of gravity of the distribution function.

**The Path Integral (Lower Level System)**

Generally, the path integral form of the kinetic equation, Eq. 6, is

\[ f_i = f_{i,0} \exp\left[-\int_0^t \nu_i dt'\right] + \int_0^t \exp\left[-\int_{t'}^t \nu_i dt''\right] G_i dt'. \tag{25} \]

This integral equation has to be solved approximately; for the one-dimensional case we introduce a grid along the axis \( x \) with the moments \( Q_i \) defined on the integer grid points \( m \), with \( x_m = m \Delta x \). At time level \( t = n \Delta t \), on the half-integer grid points \( (m + 1/2) \), the functions \( \nu_i, \nu_i^+, f_i \) are available. At the starting point \( 0 \) of the path integral these functions have to be interpolated \([1]\). A first-order predictor for point \( 1 \) on time level \((n + 1)\Delta t \) will be

\[ f_{i, n+1/2}^1 = f_{i,0}^n \exp\left[-\nu_{0,M} \Delta t\right] + \left( \frac{\nu_i^+}{\nu_i^-} \right)_0 f_{i,0,M}^n \left( 1 - \exp\left[-\nu_{0,M} \Delta t\right]\right). \tag{26} \]

To achieve a second-order accuracy, a two-point integral with piece-wise constant integrand can be used \([1]\).

Since for Eq. 21 the rhs of the equation of transfer is not exactly zero for the summational invariants, a correction step must follow. We use the condition that

\[ \sum_j \int \hat{\psi}_i \psi_j \, dc = \hat{Q}_i, \quad i = 1, \ldots, 5. \tag{27} \]

With \( f = \sum_j \sum_{k=1}^{5} \hat{f}_{ji}^d \alpha_k \hat{\psi}_k \) the coefficients \( \alpha_k \) are obtained by an iteration process, using the further restriction \( \zeta_i = \zeta_{i,d} \). Here the internal energy term is shifted from \( \hat{\psi}_5 \) into \( \hat{Q}_5 \).

**FIGURE 2.** The difference \( (T_i - T_{rot}) \) as function of time \( t \) for temperatures \( T_0 = 3, 30, 300K \) and \( \Delta j_{max} = 1, 5, 10, 20 \).
FIGURE 3. Population of the levels $j$ as function of rotational energy $j(j+1)$ for the first time steps $t = n\Delta t$, with $\Delta t = 0.02\tau_0$ and the final time step at $t_{\text{end}}$; $T_0 = 30K$, $j_{\text{max}} = 20$, $\Delta j_{\text{max}} = 20$. **Left:** At $t = 0$ all energy at level $j = 0$. **Right:** All energy initially at level $j = 10$.

The Interlaced System

With the lower and upper level equations available, the procedure for a time step is as follows: The new moments $Q_{i,m}^{n+1}$, being regarded as cell averages over a distance from $(m-1/2)$ to $(m+1/2)$, are obtained from Eq. 22 integrated over the cell

$$Q_{i,m}^{n+1} = Q_{i,m}^n + \frac{\Delta t}{2\Delta x}[F_{i,m-1/2}^n + F_{i,m+1/2}^{n+1} - F_{i,m-1/2}^{n+1} - F_{i,m+1/2}^n].$$

(28)

To be able to perform this step, $f_{j,m+1/2}^{n+1}$ must be obtained first from the path integral. Thus, the upper level is influenced through the fluxes $F_i$. The conservation of the first five moments is maintained by the global restriction imposed on the distribution function at the lower level by Eq. 27.

First Numerical Tests

To test the system, we studied a gas homogeneous in space (simplified model of nitrogen, ignoring ortho/para modifications, with $\sigma_0 = 3.58 \cdot 10^{-8} cm$, $a_2/\sigma_0 = 0.306$, $T_0 = 2.89K$, $\epsilon_2/k = 43.2K$) relaxing towards equilibrium. For this situation the fluxes $F_i$ will vanish, and therefore the upper level $Q_i$ will remain constant. Starting, for example, with a situation where all molecules are at the level $j = 0$, we can follow the redistribution of energy into the rotation taken from the translational degrees of freedom.

The cutoff $\Delta j_{\text{max}}$ of the maximum transition step has some influence upon the relaxation process when chosen too small. In Fig. 2 the relaxation of $(T_r - T_e)$ as function of $t$ is shown for $\Delta j_{\text{max}} = 1, 5, 10, 20$. We note that, with increasing energy to be redistributed and with increasing population of levels, the limit where $\Delta j_{\text{max}}$ shows no further change increases; it is also seen that only initially the relaxation process follows a change that could be modeled by the usual ansatz $dT_r/dt = -(T_r - T)/\tau_r$, with $\tau_r$ as relaxation time. During the later part of the process the approach to equilibrium is rather slow. The population of the levels $j$ is shown in Fig. 3(left) where the distributions for the first ten time steps and for the final step are plotted in the usual way. Another example is shown in Fig. 3(right): Here all molecules are initially at level $j = 10$. The relaxation towards equilibrium is rather fast in this case.

REFERENCES