

Exact nonlocal hydrodynamics predict rarefaction effects

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(Received 8 November 2024; revised 9 April 2025; accepted 25 June 2025; published 17 July 2025)

We combine the theory of slow spectral closure for linearized Boltzmann equations with Maxwell's kinetic boundary conditions to derive optimal hydrodynamics with arbitrary accommodation. Focusing on shear-mode dynamics, we obtain explicit steady state solutions in terms of Fourier integrals and closed-form expressions for the mean flow and the stress. We demonstrate that the exact nonlocal fluid model correctly predicts several rarefaction effects with accommodation, including the Couette flow and thermal creep in a plane channel.

DOI: [10.1103/4gkn-7s3x](https://doi.org/10.1103/4gkn-7s3x)

I. INTRODUCTION

Boundary effects play an important role in rarefied gas flows. Traditional no-slip boundary conditions, which assume zero relative velocity between the gas and the wall, become inadequate as the Knudsen number increases and rarefaction phenomena, such as velocity slip and temperature jump, can occur at the boundaries, thus necessitating modified boundary conditions to capture these phenomena accurately [1]. The Cercignani-Lampis model offers a more nuanced representation of gas-surface interactions by accounting for different accommodation degrees of momentum and thermal energy [2]. On a kinetic level, Maxwell's boundary conditions [3], interpolating between pure reflection and pure diffusion with an accommodation coefficient α , constitute a classical set of boundary conditions for the Boltzmann equation.

A fundamental question in kinetic theory consists in the derivation of exact hydrodynamics from kinetic model equations [4]. These are usually addressed through the Chapman-Enskog expansion and moment truncations [5]. While Grad's moment system is linearly stable, higher-order fluid models obtained through the Chapman-Enskog expansion may lead to nonphysical instabilities [6], the infamous Bobylev's instability, thus prompting the search for exact, physically consistent rarefied hydrodynamics. Along similar lines, constitutive laws for the bulk of the fluid do not necessarily give rise to natural boundary conditions for fluid-wall interactions, and higher-order slip models have to be considered on a phenomenological basis [7]. We note, however, that natural boundary conditions can be derived from moment projection models without further assumptions on gas-wall interactions [8,9]. The question of harmonization of boundary effects with higher-order fluid models is thus a largely

unsolved problem in the physics of rarefied gases when moving beyond moment projection models.

On the level of the bulk of the fluid, exact hydrodynamics have been recently derived in [10] for general near-equilibrium Boltzmann equations by projection onto the slow manifold spanned by hydrodynamic eigenvectors. These constitutive laws are dynamically optimal and globally hyperbolic. A demonstration of the dynamical optimality of a broad range of Knudsen numbers is carried out in [11]: various closure assumptions on the bulk, including Navier-Stokes and the R13 moment model [12], are compared to the spectrally closed hydrodynamics by means of Rayleigh-Brillouin scattering, thus validating its optimality. Salient features of these macroscopic field equations are their inherent spatial nonlocality, criticality in wave number and the existence of an entropy-dissipation balance. The exact nonlocal hydrodynamics thus provide a dynamically optimal description of a rarefied gas in terms of conventional macroscopic fields (density, momentum and energy) that goes way beyond the Navier-Stokes equation. In particular, any other closure assumption on higher-order moments will necessarily have larger deviations from the action moment dynamics of the underlying kinetic model [11]. We also refer to [13] for a recent spatiotemporal nonlocal fluid model for rarefied gas flows.

Let us comment on the relation of the presented exact hydrodynamic theory and Hilbert's sixth problem [4]. Classical mathematical work in kinetic theory [14–16] relates rescaled solutions to the Boltzmann equation with solutions to the Navier-Stokes equation, which are inherently limited to small Knudsen and Mach numbers. Going beyond the scaling limit of vanishing Knudsen and Mach numbers is thus a largely open direction in connection with Hilbert's sixth problem [17]. The nonlocal hydrodynamics give a somewhat different solution to Hilbert's sixth problem [18] on the linear level without any smallness assumption on Knudsen number and are equivalent to the full summation of the Chapman-Enskog series [19,20]. The current work can be interpreted as an example of how to combine dynamically optimal closure with boundary conditions, giving a more complete answer to the questions asked by Hilbert.

It is well known that characteristic properties of rarefied gas flows, such as the temperature jump or the velocity slip at

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the wall, cannot be captured by conventional hydrodynamics [7]. Analogously, the interaction of the rarefied flow with the reflective-diffusive boundary, leading to the Knudsen layer, requires higher-order hydrodynamic models [21] or kinetic simulations [22]. We also refer to [23] for a recent treatment of thermo-osmotic effects in connection with gas-wall interactions derived from general fluctuations-dissipation theory for inhomogeneous systems.

In this work, we extend the exact nonlocal fluid equations by incorporating kinetic boundary conditions. We provide a general solution method and demonstrate that criticality is the dominant feature responsible for rarefaction effects. While our methodology applies to the full nonlocal hydrodynamics, we demonstrate it by focusing on problems which only include the shear mode, thus allowing for an effectively one-dimensional kinetic modeling. The nonlocal hydrodynamics with accommodation are exemplified with two classical rarefaction problems, planar Couette flow and thermal creep, for which tabulated solutions for the stresses and flow rates have been calculated for the Bhatnagar-Gross-Krook (BGK) collision model [24,25]. We remark that the BGK model, although widely used in kinetic theory, has Prandtl number one (as opposed to the physical $\text{Pr} = 2/3$), while retaining important features of the full Boltzmann equation, such as collision invariants and the H theorem. We stress at this point that the theory presented in the following can be applied directly to the full linear Boltzmann equation and that the BGK model has been chosen as a minimal working example for which the operator spectral calculations can be carried out explicitly. We further stress that similar arguments apply to the Shakhov model with tunable Prandtl number, including the physically relevant case of $\text{Pr} = 2/3$, for which a full explicit spectral analysis has been carried out in [26].

II. EXACT HYDRODYNAMICS AND KINETIC BOUNDARY CONDITIONS

In the following, we focus on linear rarefied flow problems to illustrate how the underlying spectral closure technique can be combined with kinetic boundary conditions. In particular, we exclude turbulent flow phenomena from the current analysis, for which nonlinear effects are vital [27], and focus on stationary flows. In fact, the linear flow regime is sufficient to capture rarefaction effects, such as the Knudsen minimum or the temperature jump [1].

Consider the following nonlocal hydrodynamic model in frequency space,

$$\partial_t \hat{u}(k) = \hat{\lambda}(k) \hat{u}(k), \quad (1)$$

where $\hat{u}$ is the spatial Fourier transform of the velocity field u and $\hat{\lambda}(k)$ is the frequency-dependent shear-type mode of the underlying Boltzmann operator, acting as a Fourier multiplier [10,28]. Equation (1) was first derived in [29] from the dynamically optimal hydrodynamic closure applied to the one-dimensional kinetic equation. In physical space, Eq. (1) defines a pseudodifferential evolution equation for the shear velocity u with the Fourier multiplier $\hat{\lambda}$ acting through spatial convolution with an integral kernel.

The Fourier multiplier satisfies the asymptotics,

$$\hat{\lambda}(k) = \mathcal{O}(k^2), \quad k \rightarrow 0, \quad (2)$$

corresponding to the Navier-Stokes limit in consistency with the Chapman-Enskog expansion, while it remains bounded for $k \rightarrow \infty$. Indeed, there exists a critical wave number k_{crit} such that $\hat{\lambda}(k)$ exists as an isolated eigenvalue only for $|k| < k_{\text{crit}}$, see [10], and we set

$$\hat{\lambda}(k) = -\nu, \quad |k| > k_{\text{crit}} \quad (3)$$

as an extension of the shear-type mode in frequency space, where ν is the collision frequency of the underlying kinetic model evaluated at $\mathbf{v} = 0$, see [30]. The extension of the hydrodynamic mode (3) can thus be interpreted as a way to include information about the essential spectrum of the Boltzmann kinetic equation into the nonlocal hydrodynamics.

Equation (1) is based on an underlying kinetic operator of Boltzmann type in frequency space, $\mathcal{L}_k = -i\mathbf{k} \cdot \mathbf{v} + \mathcal{Q}$, where $\mathcal{Q}$ is a self-adjoint collision operator, see [10]. In this work, we restrict our analysis to one spatial dimension and assume that the velocity field is aligned with the shear flow direction. Taking problem-specific moments in velocities then leads to a one-dimensional kinetic operator in frequency space of the form $L_k = -ikv + \mathcal{Q}_s$ and a one-dimensional distribution function $f(x, v)$, where $\mathcal{Q}_s$ is the self-adjoint projected collision operator, in the shear direction [31]. The nonlocal evolution equation (1) is then derived from the projection onto the hydrodynamic slow manifold,

$$f_{\text{hydro}}(x, v) = \frac{1}{\sqrt{2\pi}} \int dk \hat{f}_\lambda(v, k) \hat{u}(k) e^{ikx}, \quad (4)$$

where $\hat{f}_\lambda$ is the eigenfunction of L_k with eigenvalue $\hat{\lambda}$, indexed by wavenumber.

Below, we use units such that the thermal speed is

$$v_T = \sqrt{k_B T / m} = 1 \quad (5)$$

and the global Maxwellian is

$$f^{\text{eq}}(v) = (1/\sqrt{2\pi}) \exp(-v^2/2). \quad (6)$$

The general reflective-diffusive boundary conditions [30] for a one-dimensional kinetic equation on the interval of length L take the form

$$\begin{aligned} f(0, v) - (1 - \alpha)f(0, -v) &= \phi_0(v, \alpha), \quad v > 0, \\ f(L, -v) - (1 - \alpha)f(L, v) &= \phi_L(v, \alpha), \quad v > 0, \end{aligned} \quad (7)$$

where L is the distance between the walls of the channel, $0 \leq \alpha \leq 1$ is the accommodation coefficient, and the polynomials $\phi_{0,L}$ are derived from the equilibrium distributions at the respective walls by taking velocity moments accordingly [31].

III. EXPLICIT STEADY STATE SOLUTIONS

To derive a steady state solution to (1) between the two plates, we first observe that any information that defines a nontrivial steady state has to be confined to the boundary points. A classical result in distribution theory [32] implies that the boundary data has to be a superposition of two delta distributions and their derivatives. We will consider only the leading order contribution of these boundary functions,

thus assuming two delta functions of opposing sign at the respective boundaries, which leads to the equation,

$$\int_{-\infty}^{\infty} dy \int_{-\infty}^{\infty} dk u(x-y) \hat{\lambda}(k) e^{ikx} = \bar{\sigma} (\delta(x-L) - \delta(x)), \quad (8)$$

where δ is the Dirac delta function and where the connection of the parameter $\bar{\sigma}$ to the stress component will become apparent later. We emphasize that the inclusion of higher-order derivatives of delta distributions at the boundary will improve the fit to the steady state solution close to the walls. Since these effects become more dominant for narrower channels, we expect that the inclusion of higher-order boundary functions will improve the fit of the spectrally closed hydrodynamics to the full BGK results for larger Knudsen numbers. The leading-order approximation with two delta functions, however, is sufficient to illustrate the main computation strategy in this paper.

Equation (8) can now readily be solved in Fourier space via division by $\hat{\lambda}$ and addition of an integration constant. The explicit steady state solution to Eqs. (1) and (8), respectively, on the interval $(0, L)$ is then given by

$$u(x) = \bar{u} + \frac{\bar{\sigma}}{2\pi} \int_{-\infty}^{\infty} dk \frac{(e^{-iLk} - 1)}{\hat{\lambda}(k)} e^{ikx}, \quad (9)$$

for the mean flow component $\bar{u}$ and the constant stress component $\bar{\sigma}$.

The integral expression in (9) has to be interpreted as a principal value for small wave numbers, whose convergence is guaranteed by the asymptotics (2). Indeed, the choice of delta functions with opposing sign guarantees that the numerator in (9) is of order $\sim k$, thus implying that the integrand is of order $\sim k^{-1}$. A contour-integration argument then shows that (9) exists for k small enough. For large wave numbers, the integral does not converge in the classical sense as the inverse Fourier transform of a bounded signal and has to be interpreted as a generalized function. We can thus rewrite (9) as

$$u(x) = \bar{u} + \frac{\bar{\sigma}}{2\pi} \int_{-k_{\text{crit}}}^{k_{\text{crit}}} dk \left(\frac{1}{\hat{\lambda}(k)} + \frac{1}{v} \right) (e^{-iLk} - 1) e^{ikx} + \frac{\bar{\sigma}}{2\pi v} (\delta(x) - \delta(x-L)). \quad (10)$$

We emphasize the inherently weak character of the steady state solution to (1), which splits into a smooth part, the first two terms in (10), and a distributional part due to the boundedness of $\hat{\lambda}$ by (3). In the limit $\text{Kn} \rightarrow 0$, however, solution (9) converges to the classical steady-state solution of the heat equation, since both the collision frequency ν as well as the critical wave number k_{crit} go to infinity, thus proving consistency with the Chapman-Enskog expansion.

While the Fourier multiplier $\hat{\lambda}$ is defined for all frequencies and hence on the whole real line, solution (9) only uses information inside the interval $(0, L)$ and at its boundary. Indeed, the steady state solution (10) becomes singular at the boundary, while its smooth component can be extended to the real line. This phenomenon is reminiscent of the tunneling effect in quantum mechanics [33]. We stress that all these properties are consequences of the nonlocal character of (1). Furthermore, on the slow manifold, the stress is related to the

velocity field via the Fourier multiplier [10],

$$\hat{\sigma}(k) = -\frac{\hat{\lambda}(k)}{ik} \hat{u}(k). \quad (11)$$

From the asymptotics (2), we necessarily have that $\hat{\sigma}(k) = \mathcal{O}(k)$, while the application of (11) to the explicit solution (9) implies that

$$\sigma(x) = \bar{\sigma}, \quad 0 < x < L. \quad (12)$$

Thus, the steady state solution is defined by (10) up to the two constants, the mean flow $\bar{u}$, and the stress $\bar{\sigma}$. The latter are derived from the kinetic boundary conditions (7), where we have to balance the corresponding first-order fluxes on the hydrodynamic slow manifold [34]. To that end, we multiply both equations in (7) with v and integrate over non-negative velocities. Restricting the distribution function appearing on the left-hand side of (7) to the hydrodynamic slow manifold (4) and taking half-space fluxes accordingly leads to the Fourier multiplier

$$\hat{s}(k) = \frac{1}{\sqrt{2\pi}} \int_0^{\infty} dv e^{-\frac{v^2}{2}} v \hat{f}_{\lambda}(v, k). \quad (13)$$

The multiplier (13) satisfies the symmetry

$$\hat{s}(-k) = \hat{s}^*(k), \quad (14)$$

which follows from the general symmetry of the shear-mode eigenvectors [10,28]

$$\hat{f}_{\lambda}(v, -k) = \hat{f}_{\lambda}^*(v, k). \quad (15)$$

Similarly, by taking half-space fluxes for the boundary functions on the right-hand side of (7), we obtain

$$\sigma_{0,L}(\alpha) = \frac{1}{\sqrt{2\pi}} \int_0^{\infty} dv e^{-\frac{v^2}{2}} v \phi_{0,L}(v, \alpha). \quad (16)$$

Combining (13) with (16), we arrive at a linear system for the mean flow $\bar{u}$ and the flux $\bar{\sigma}$,

$$\begin{pmatrix} \alpha & \eta(L) \\ \alpha & -\eta(-L) \end{pmatrix} \begin{pmatrix} \bar{u} \\ \bar{\sigma} \end{pmatrix} = \begin{pmatrix} \sigma_0 \\ \sigma_L \end{pmatrix}, \quad (17)$$

where we have defined the coefficient function

$$\eta(L) = 2\text{Re} \int_0^{\infty} dk \frac{(1 - e^{-iLk})}{\hat{\lambda}(k)} [\hat{s}(k) - (1 - \alpha)\hat{s}^*(k)], \quad (18)$$

and have omitted the dependence on α to ease notation.

System (17) has a unique solution provided that $\alpha \neq 0$. Indeed, it is well known that for purely reflective boundaries ($\alpha = 0$), the mean-flow component cannot be recovered uniquely from the boundary conditions [35]. This property is also reflected on the level of the hydrodynamic manifold (4), which satisfies the symmetry (15). The solution to (17) is given explicitly by

$$\bar{u} = \frac{\sigma_0 \eta(-L) + \sigma_L \eta(L)}{\alpha [\eta(-L) + \eta(L)]}, \quad \bar{\sigma} = \frac{\sigma_0 - \sigma_L}{\eta(-L) + \eta(L)} \quad (19)$$

whenever $\alpha \neq 0$, thus expressing the mean flow and the flux in terms of the width of the channel L and Maxwell's accommodation coefficient α . Thus, the solution to the steady-state problem is reduced to quadratures (18) for a generic Boltzmann equation.

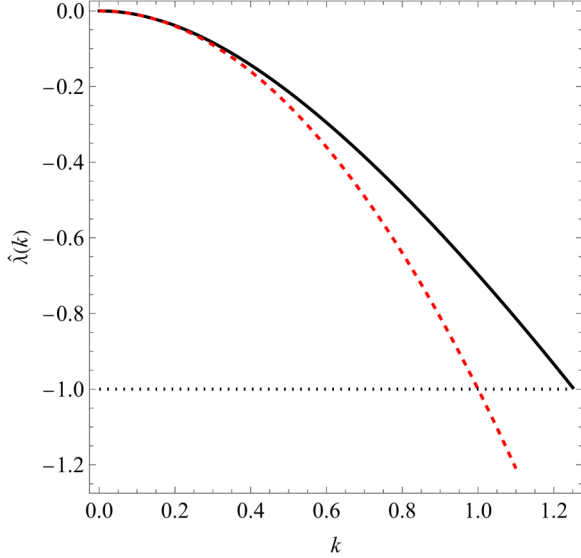


FIG. 1. The shear mode Fourier multiplier (solid black line) as derived from the spectral analysis of the BGK equation. Note that $\hat{\lambda}$ is compactly supported in frequency space with critical wave number $k_{\text{crit}} = \sqrt{\pi/2}\tau^{-1}$ (where τ is the global relaxation time of the BGK model, normalized to one here). The red dashed line shows the dissipation relation of the Navier-Stokes equation $-k^2$ in comparison.

IV. EVALUATE AND COMPARISON FOR THE ONE-DIMENSIONAL BGK EQUATION

To assess the accuracy of the nonlocal hydrodynamics, we compare (19) to numerical solutions of the Bhatnagar-Gross-Krook (BGK) kinetic equation [36]. For a complete and explicit spectral theory of the linear BGK operator, we refer to [28]: The eigenfunction associated to the shear mode takes the form

$$f_{\hat{\lambda}}(v, k) = \frac{1}{1 + i\tau kv + \tau \hat{\lambda}(k)}, \quad (20)$$

where $\tau = 1/\nu$ is the relaxation time of the BGK equation. Furthermore, the BGK shear mode $\hat{\lambda}$ is the solution to the equation [28]

$$Z\left(i\frac{\tau \hat{\lambda} + 1}{\tau k}\right) = i\tau k, \quad (21)$$

where $Z(\zeta) = Z^+(\zeta) - Z^+(-\zeta)$ is the plasma dispersion function and

$$Z^+(\zeta) = \frac{1}{\sqrt{2\pi}} \int_0^\infty dv \frac{e^{-v^2/2}}{v - \zeta} \quad (22)$$

is the incomplete plasma dispersion function [37], while the critical wave number of the shear mode is

$$k_{\text{crit}} = \sqrt{\frac{\pi}{2}} \frac{1}{\tau}. \quad (23)$$

The shear mode Fourier multiplier $\hat{\lambda}$ is depicted in Fig. 1. We consider Eq. (1) on the interval $x \in (0, L)$ and define the Knudsen number as

$$\text{Kn} = \frac{\tau}{L}, \quad (24)$$

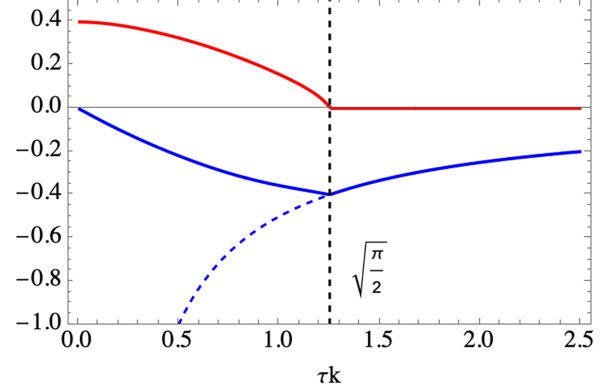


FIG. 2. Real part (red) and imaginary part (blue) of the Fourier multiplier $\hat{s}$ for the BGK model (25). For $k\tau > \sqrt{\pi/2}$ [critical wave number (23), dashed vertical line], the real part vanishes while the imaginary part becomes $-\frac{1}{2k\tau}i$ (dashed blue line).

recalling that we have chosen units such that $v_T = 1$. For the BGK shear mode, the Fourier multiplier (13) takes explicit form

$$\hat{s} = \frac{1}{2ik\tau} + \frac{\tau \hat{\lambda} + 1}{\tau^2 k^2} Z^+\left(i\frac{\tau \hat{\lambda} + 1}{\tau k}\right). \quad (25)$$

Function (25) is shown in Fig. 2.

First we consider the rarefied planar Couette flow generated by the viscous forces of two parallel plates moving in opposite directions. In this case [25],

$$\phi_0(v, \alpha) = \alpha, \quad \phi_L(v, \alpha) = -\alpha. \quad (26)$$

The normalized stress [31] is derived from the explicit $\bar{\sigma}$ solution (19) as

$$P_{xz} = \frac{2\pi\alpha}{\sqrt{2}[\eta(L) - \eta(-L)]}. \quad (27)$$

Figure 3 shows a comparison of (27) to numerical results of the full BGK kinetic equation, indicating excellent agreement up to Knudsen numbers $\text{Kn} \sim \mathcal{O}(10)$. The coefficient function

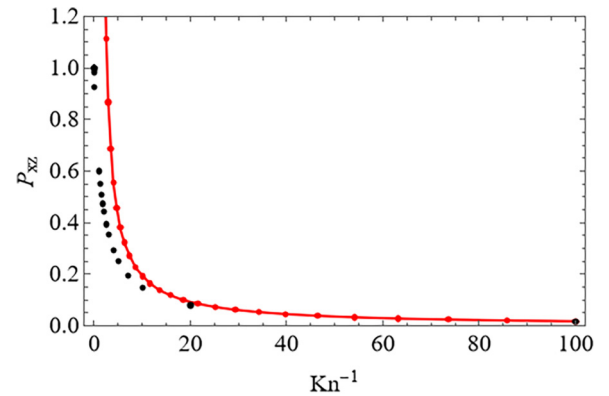


FIG. 3. Normalized stress for the planar Couette flow ($\tau = 1$, $\alpha = 1$). Solid red line with markers: present rarefied hydrodynamics; Black markers: tabulated numerical calculation for the BGK model [25].

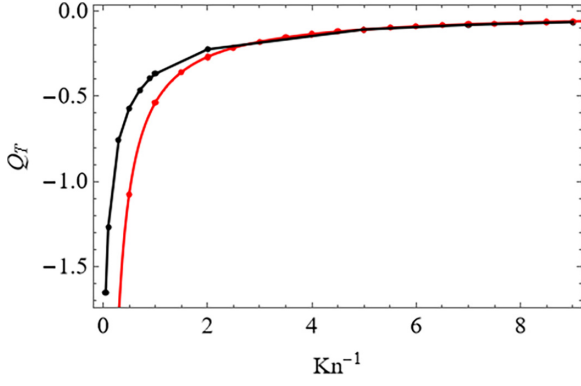


FIG. 4. Normalized flow rate for the thermal creep flow ($\tau = 1$, $\alpha = 0.5$). Solid red line with markers present rarefied hydrodynamics; Black markers are tabulated numerical calculation for the BGK model [25].

(18) satisfies the asymptotics

$$\begin{aligned} \eta(L) &= \left(\frac{\hat{s}(0)}{\tau} \int_0^\infty dy \frac{1 - e^{-iy}}{y^2} \right) L + \mathcal{O}(L^2) \\ &= \sqrt{2\pi} \frac{L}{\tau} + \mathcal{O}(L^2), \quad L \rightarrow \infty, \end{aligned} \quad (28)$$

where we have used the asymptotics $\hat{\lambda}(k) = -\tau k^2 + \mathcal{O}(k^4)$, $k \rightarrow 0$, of the BGK shear mode together with $\hat{s}(0) = 1/\sqrt{2\pi}$. Combining (28) with (27) gives

$$P_{xz} = \sqrt{\pi} \frac{\tau}{L} + \mathcal{O}(L^{-2}), \quad L \rightarrow \infty, \quad (29)$$

which is consistent with the Navier-Stokes asymptotics of the planar Couette flow, see [24]. Let us remark that the normalized flow rate obtained from the spectrally closed hydrodynamics starts to deviate from the BGK reference curve at around $\text{Kn} \approx 10$. Since the current calculations only consider the leading-order contributions of the wall, we assume that the inclusion of higher derivatives in the boundary functions (8) will increase the accuracy for higher Knudsen numbers, at which the boundary effects become more pronounced.

As a second example, we consider the thermal creep problem, for which

$$\phi_0(v, \alpha) = \phi_L(v, \alpha) = \frac{\alpha}{2} \left(v^2 - \frac{1}{2} \right); \quad (30)$$

see [25]. The macroscopic quantity of interest is the normalized flow rate,

$$Q_T(L) = -\frac{2\tau}{L^2} \int_0^L dx u(x). \quad (31)$$

The explicit solution (19) predicts a vanishing flux $\bar{\sigma}$, while it recovers the mean flow component as

$$\bar{u} = \frac{1}{4\sqrt{2\pi}} \int_0^\infty dv v(2v^2 - 1) e^{-\frac{v^2}{2}} = \frac{3}{4\sqrt{2\pi}}, \quad (32)$$

and the normalized flow rate as

$$Q_T(L) = -\frac{2\tau}{L} \bar{u} = -\frac{3}{2\sqrt{2\pi}} \frac{\tau}{L}. \quad (33)$$

Figure 4 shows a comparison of (33) to numerical results of the full BGK kinetic equation, indicating excellent agreement up to Knudsen numbers $\text{Kn} \sim \mathcal{O}(1)$. Similar to the previous example, we expect an improved fit for larger Knudsen numbers through the inclusion of higher-order boundary terms.

V. CONCLUSION

We conclude with a summary of the results. We presented an extension of the exact rarefied hydrodynamics [10] by general kinetic boundary conditions. We provided a closed-form solution to a class of rarefied flow problems with general accommodation and showed a quantitative comparison for the planar Couette flow and the thermal creep, giving excellent agreement over a remarkably wide range of Knudsen numbers. Thus, the practical solution to Hilbert's sixth problem [18] on the linear level has been extended to include boundary conditions as well. We demonstrated that rarefaction effects are solely a consequence of the nonlocality of exact hydrodynamics, a feature which is not shared by any approximate hydrodynamics such as Navier-Stokes or Burnett [5]. While the hydrodynamics for the bulk are exact, the current treatment gives exact formulas for the mean flow and the stress component of the velocity field by matching two moments at the boundary. However, we expect that inclusion of higher-order moments in the kinetic boundary condition (7) will improve the result even further. This line of research will be tackled in a forthcoming work, along with a comparative study of the presented approach to higher-order slip models and extended hydrodynamics with boundary conditions.

Finally, while we focus on the shear mode dynamics in this work, the above approach is applicable to general nonlocal hydrodynamics for the full set of modes [10]. We plan to give a broader comparison of macroscopic flow properties such as the velocity field and the Knudsen layer function, along the lines of [38] in a forthcoming paper as well. Furthermore, extension to nonlinear flow problems, such as rarefied turbulence, with appropriate boundary conditions will be pursued as well.

ACKNOWLEDGMENTS

This work was supported by European Research Council (ERC) Advanced Grant No. 834763-PonD and Swiss National Science Foundation (SNSF) Grant No. 200021-228065. Computational resources at the Swiss National Super Computing Center CSCS were provided under the Grant No. s1286.

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