Knudsen Layers from Moment Equations

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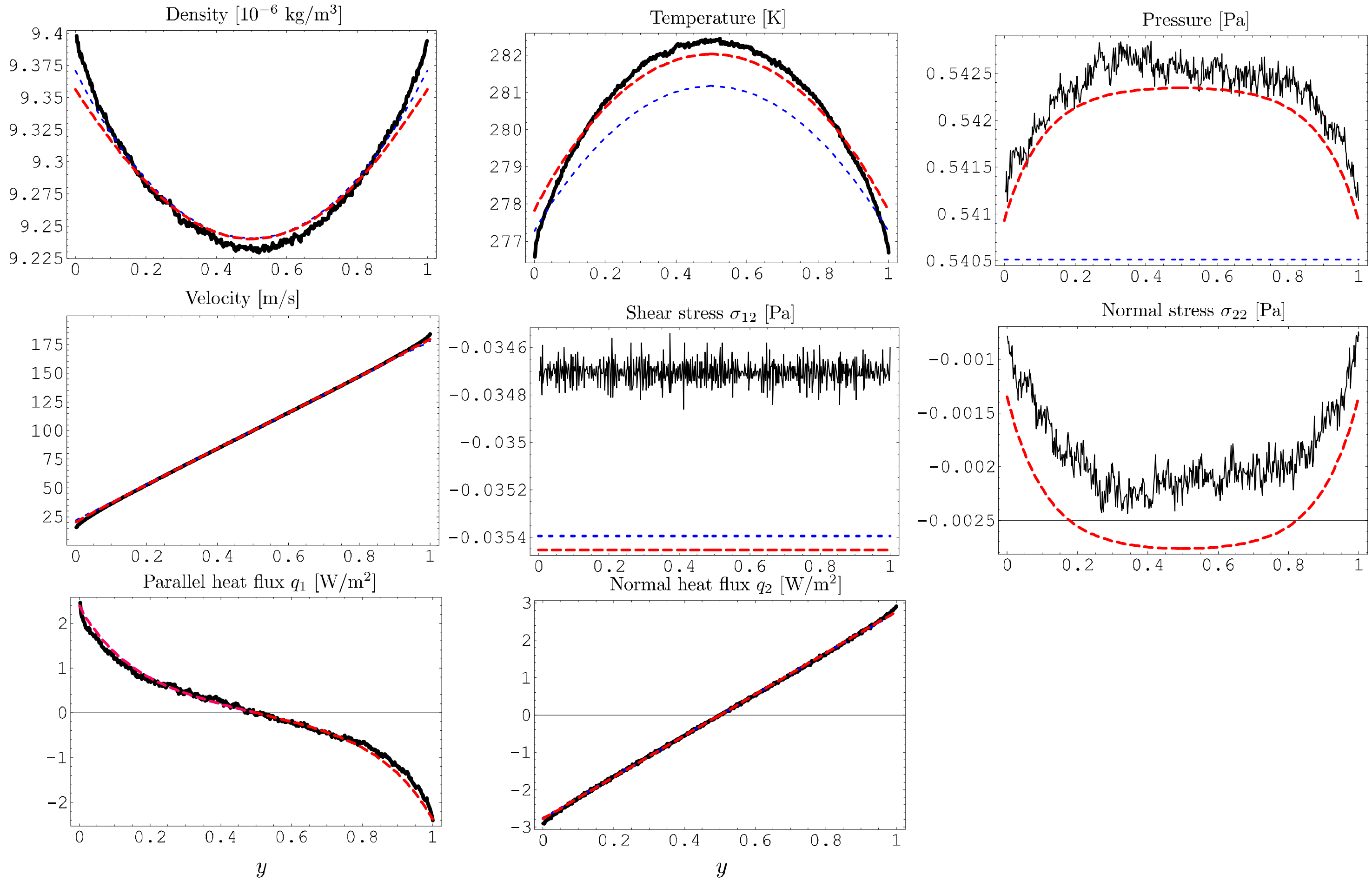
Knudsen layers in microscale transport

e.g., Couette flow in ideal gases



black: DSMC **blue:** Navier-Stokes-Fourier **red:** R13 equations

Knudsen layers: dominate in linear flows (for not too small Knudsen numbers)

not too important in strongly non-linear flows

Knudsen layers and moments?

Moments are superposition of many Knudsen layers [HS 2002]

Question: How many Knudsen layers / moment equations required?

Answer: use simple linear kinetic model

$\Rrightarrow$ analytical calculations for all moment numbers

The kinetic model and its properties

kinetic model for 1-D heat transfer (simplified phonon/photon model)

$$\frac{\partial f}{\partial t} + \mu \frac{\partial f}{\partial x} = -\frac{1}{\varepsilon}\left(f - \frac{1}{2}\lambda_0\right)$$

$f(x,t,\mu)$ - distribution function, ε- Knudsen number, $\mu = \cos\vartheta$ - direction cosine

energy density and heat flux are moments

$$\lambda_0(x,t) = \int_{-1}^{1} f(x,t,\mu)\, d\mu \quad , \quad \lambda_1(x,t) = \int_{-1}^{1} \mu f(x,t,\mu)\, d\mu$$

energy is conserved

$$\frac{\partial \lambda_0}{\partial t} + \frac{\partial \lambda_1}{\partial x} = 0$$

H-theorem

$$\frac{\partial \eta}{\partial t} + \frac{\partial \phi}{\partial x} = \sigma \geq 0$$

entropy density, flux, generation

$$\eta = -\frac{1}{2}\int_{-1}^{1} f^2 d\mu \ , \ \phi = -\frac{1}{2}\int_{-1}^{1} \mu f^2 d\mu \ , \ \sigma = \frac{1}{\varepsilon}\int_{-1}^{1}\left(f - \frac{\lambda_0}{2}\right)^2 d\mu$$

Moments and their equations

N **moments of Legendre polynomials**

$$\lambda_n = \int_{-1}^{1} P_n(\mu) f d\mu \qquad (n = 0, 1, \ldots, N)$$

P_N **- approximation of distribution**

$$f^{(N)} = \sum_{n=0}^{N} \left(n + \frac{1}{2}\right) P_n(\mu) \lambda_n$$

moment equations from $f^{(N)}$ and kinetic equation

$$\frac{\partial \lambda_0}{\partial t} + \frac{\partial \lambda_1}{\partial x} = 0$$

$$\frac{\partial \lambda_n}{\partial t} + \frac{n}{2n+1}\frac{\partial \lambda_{n-1}}{\partial x} + \frac{n+1}{2n+1}\frac{\partial \lambda_{n+1}}{\partial x} = -\frac{1}{\varepsilon}\lambda_n$$

$$\frac{\partial \lambda_N}{\partial t} + \frac{N}{2N+1}\frac{\partial \lambda_{N-1}}{\partial x} = -\frac{1}{\varepsilon}\lambda_N$$

Question: what value of N for Knudsen number ε ??

H-theorem for moments

P_N approximation gives second law

$$\frac{\partial \eta}{\partial t} + \frac{\partial \phi}{\partial x} = \sigma \geq 0$$

with quadratic expressions

$$\eta = -\frac{1}{2} \sum_{n=0}^{N} \left(n + \frac{1}{2} \right) \lambda_n^2$$

$$\phi = -\sum_{n=0}^{N-1} \frac{n+1}{2} \lambda_n \lambda_{n+1}$$

$$\sigma = \frac{1}{\varepsilon} \sum_{n=1}^{N} \left(n + \frac{1}{2} \right) \lambda_n \lambda_n$$

Remark: Quadratic entropy for R13 eqs. [HS & MT 2007]

Boundary conditions

Maxwell boundary conditions for distribution function ($f_W = \frac{1}{2}\lambda_W$)

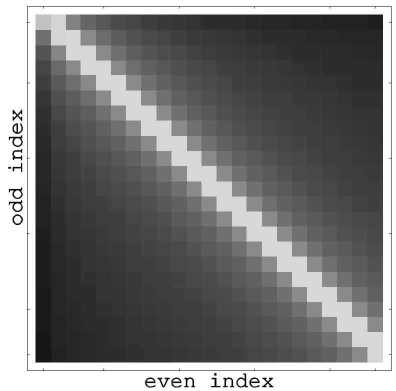
$$\bar{f} = \begin{cases} \chi f_W + (1-\chi)\, f\,(-\gamma\mu) & \gamma\mu > 0 \\ \\ f\,(\gamma\mu) & \gamma\mu < 0 \end{cases}$$

χ - accommodation coefficient, $\gamma = \pm 1$ at $x = \mp 1/2$

boundary conditions for moments: use odd moments only! [Grad 1949]

$$\bar{\lambda}_n = -\gamma \Psi_{n0} \left[\bar{\lambda}_0 - \lambda_W\right] - \gamma \sum_{m=2}^{N} \Psi_{nm} \bar{\lambda}_m \qquad (n \text{ odd, } m \text{ even})$$

$$\Psi_{nm} = \frac{2\chi}{2-\chi}\left(m + \frac{1}{2}\right) \int_0^1 P_n(\mu)\, P_m(\mu)\, d\mu$$



Remark: H-theorem at walls fulfilled, computation via entropy fluxes

Asymptotics: Chapman-Enskog expansion

expansion in Knudsen number only non-conserved moments

$$\lambda_n = \sum_{\alpha=0} \varepsilon^\alpha \lambda_n^{(\alpha)} \quad (n \geq 1)$$

zeroth order contributions vanish

$$\lambda_n^{(0)} = 0 \quad (n \geq 1)$$

only heat flux has first order contribution (Fourier's law)

$$\lambda_1^{(1)} = -\frac{1}{3}\frac{\partial \lambda_0}{\partial x} \quad , \quad \lambda_n^{(1)} = 0 \quad (n \geq 2) \ .$$

n-th **moment has order** n

$$\lambda_n^{(\alpha-1)} = 0 \text{ for } \alpha \leq n$$

e.g., third order transport eq.

$$\frac{\partial \lambda_0}{\partial t} - \frac{1}{3}\varepsilon \frac{\partial^2 \lambda_0}{\partial x^2} + \varepsilon^3 \frac{1}{45}\frac{\partial^3 \lambda_0}{\partial x^4} = 0$$

expansion only valid in bulk – not in Knudsen layer

Asymptotics: order of magnitude method

based on CE order of magnitude

$$\lambda_n = \varepsilon^n \tilde{\lambda}_n$$

step by step reduction to order $\mathcal{O}\left(\varepsilon^{2N}\right)$ yields truncated set [Leicester 2005]

$$\frac{\partial \lambda_0}{\partial t} + \frac{\partial \lambda_1}{\partial x} = 0$$

$$\frac{\partial \lambda_n}{\partial t} + \frac{n}{2n+1}\frac{\partial \lambda_{n-1}}{\partial x} + \frac{n+1}{2n+1}\frac{\partial \lambda_{n+1}}{\partial x} = -\frac{1}{\varepsilon}\lambda_n \ \ (n = 1, \ldots, N-1)$$

$$\frac{\partial \lambda_N}{\partial t} + \frac{N}{2N+1}\frac{\partial \lambda_{N-1}}{\partial x} = -\frac{1}{\varepsilon}\lambda_N$$

expansion only valid in bulk – not in Knudsen layer

Moment system as discrete velocity model

N-**moment equations in matrix form**

$$\frac{\partial \lambda_m}{\partial t} + \mathcal{A}_{mn} \frac{\partial \lambda_n}{\partial x} = \mathcal{C}_{mn} \lambda_n$$

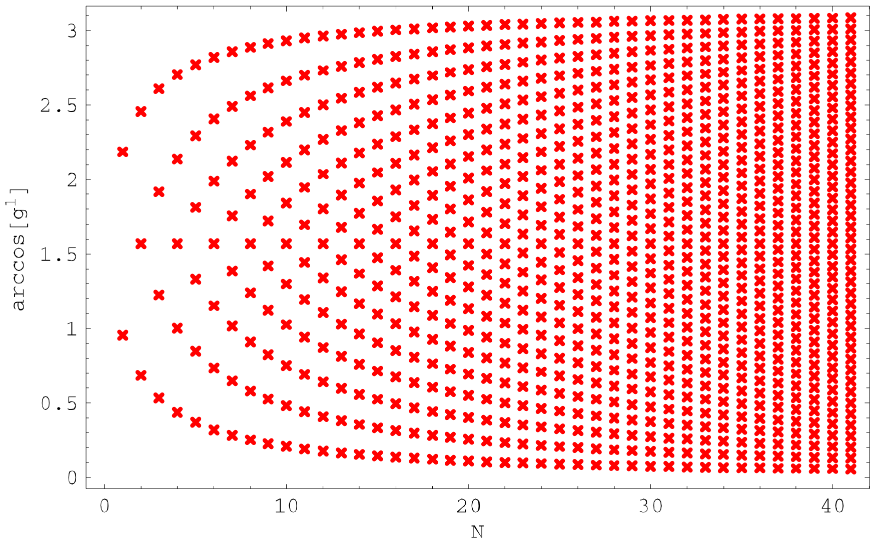
diagonalize

$$\frac{\partial \gamma_l}{\partial t} + g^{(l)} \frac{\partial \gamma_l}{\partial x} = -\frac{1}{\varepsilon} \gamma_l + \frac{1}{\varepsilon} \theta_{l0}^{-1} \theta_{0r} \gamma_r$$

$g^{(l)}$ - eigenvalues, θ_{mn} - matrix of eigenvectors, γ_n - population numbers, $\lambda_n = \theta_{nr} \gamma_r$ - org. moments

eigenvalues correspond to discrete angles evenly distributed in $[0, \pi]$

$$g^{(l)} = \mu^{(l)} = \cos \vartheta^{(l)}$$



Question: Is there similar analogy for 3-D moment eqs??

Knudsen layer solutions (steady state)

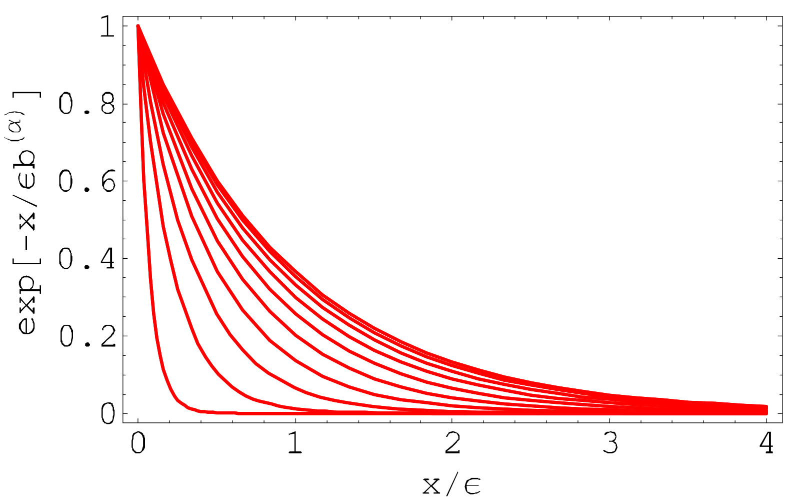
bulk moments

$$\lambda_0 = K - \frac{3}{\varepsilon}\lambda_1 x - 2\lambda_2 \quad , \quad \lambda_1 = const.$$

Knudsen layer moments

$$\lambda_n = \sum_{m=2} \Phi_{nm}\Gamma_m^0 \exp\left[-\frac{x}{\varepsilon b^{(m)}}\right] \quad (n \geq 2)$$

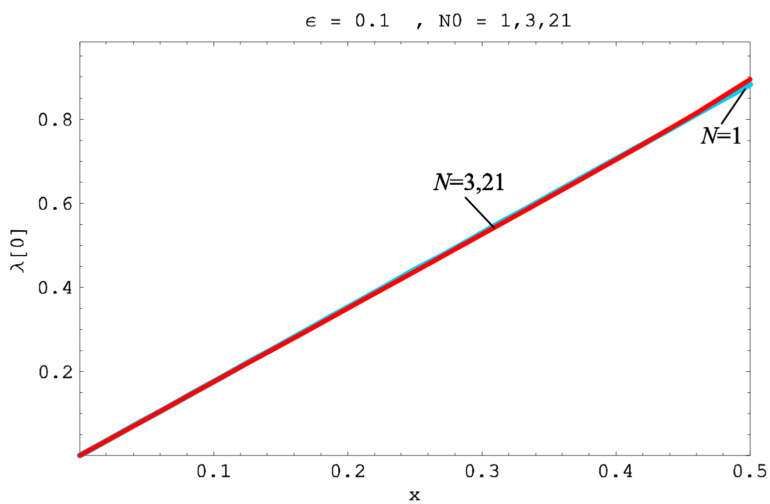
$b^{(m)}$, Φ_{nm} - eigenvalues/vectors of $\mathcal{B}_{nm} = \frac{n+1}{2n+3}\delta_{n,m-1} + \frac{n+2}{2n+3}\delta_{n,m+1}$



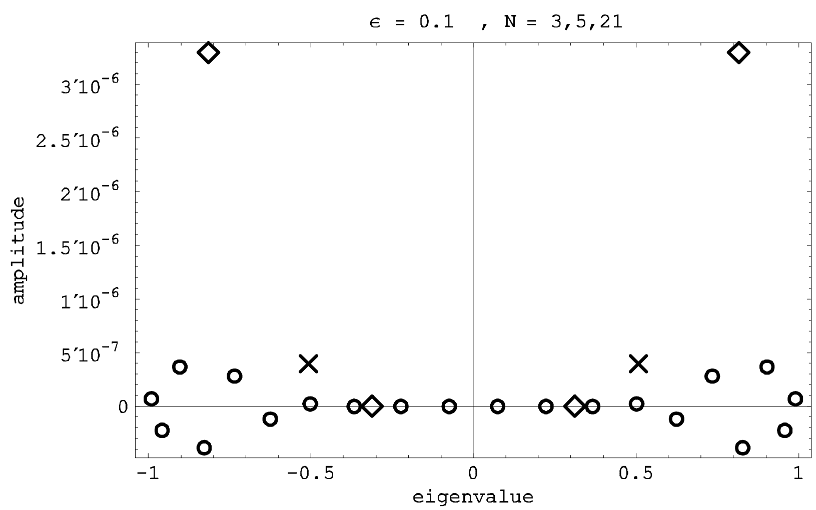
constants of integration K, λ_1, Γ_m^0 from jump boundary conditions with $\lambda_W\left(\pm\frac{1}{2}\right) = \pm 1$

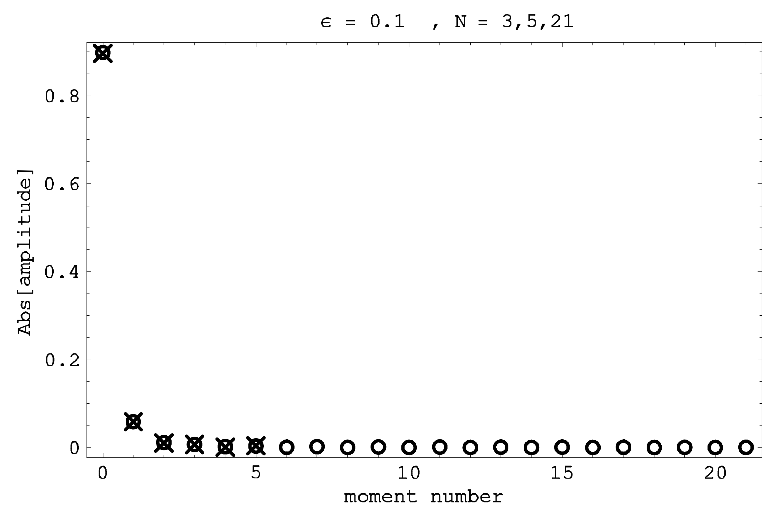
Results for $\varepsilon = 0.1$ $(N = 1, 3, 5, 21)$

energy density



eigenvalues/amplitudes and moments



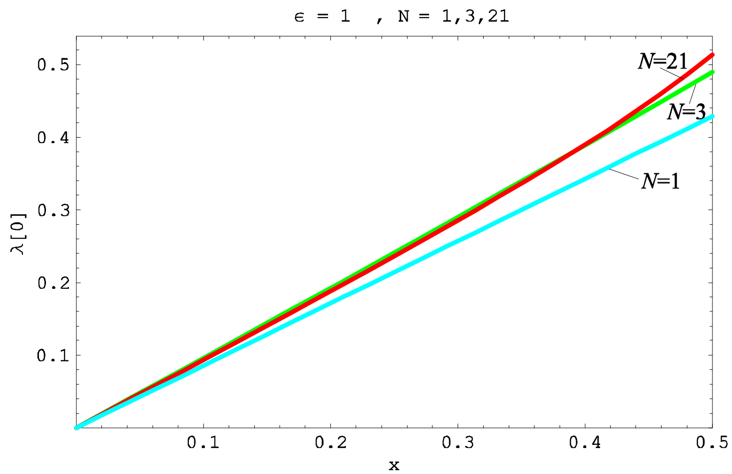


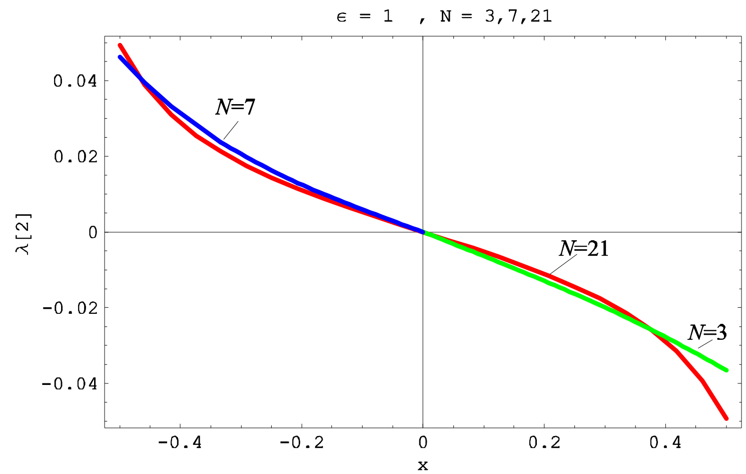
jumps, invisible Knudsen layers, no visible differences with N

Results for $\varepsilon = 1$ $(N = 1, 3, 7, 21)$

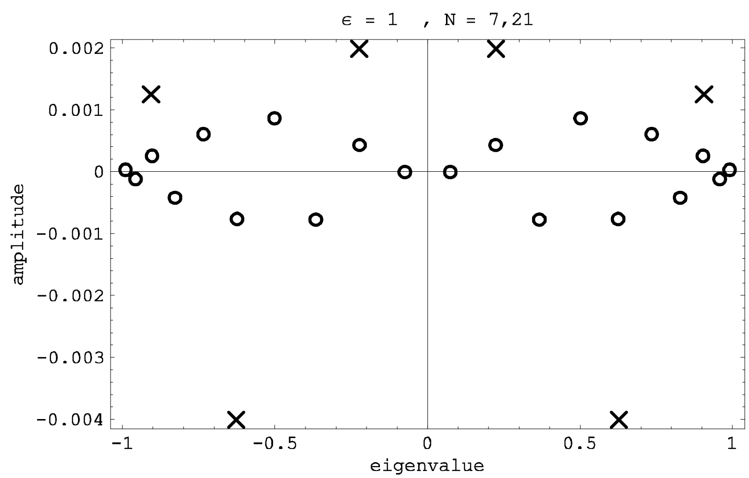
$N = \{1, 3, 7, 21\}$: heat flux:$\lambda_1 = \{-0.2857, -0.2779, 0.2770, -0.2767\}$

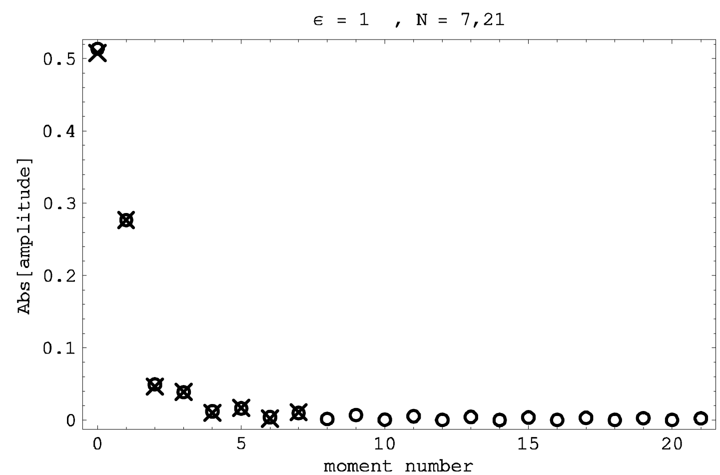
energy density





eigenvalues/amplitudes and moments

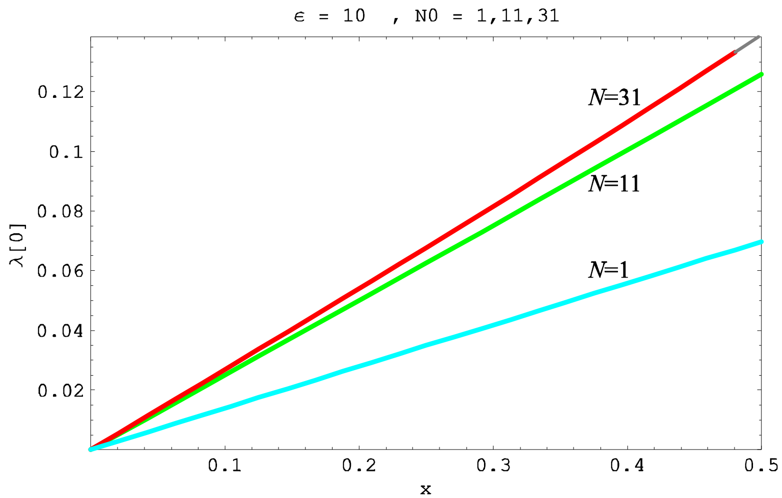




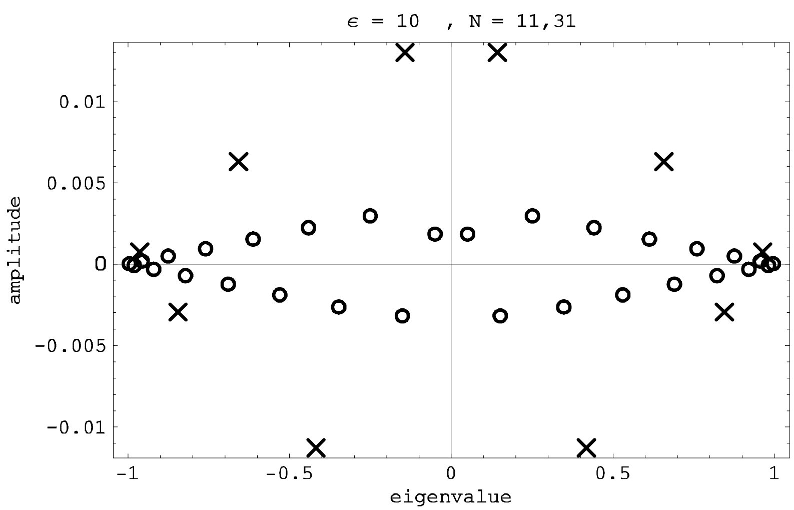
marked Knudsen layers, already $N = 3$ gives good agreement!!

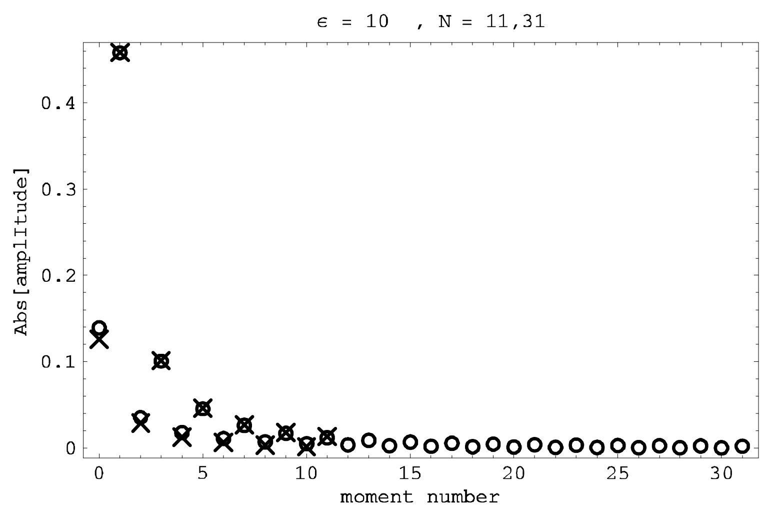
Results for $\varepsilon = 10$ $(N = 1, 11, 31)$

Energy density, second moment



Eigenvalues/amplitudes and moments

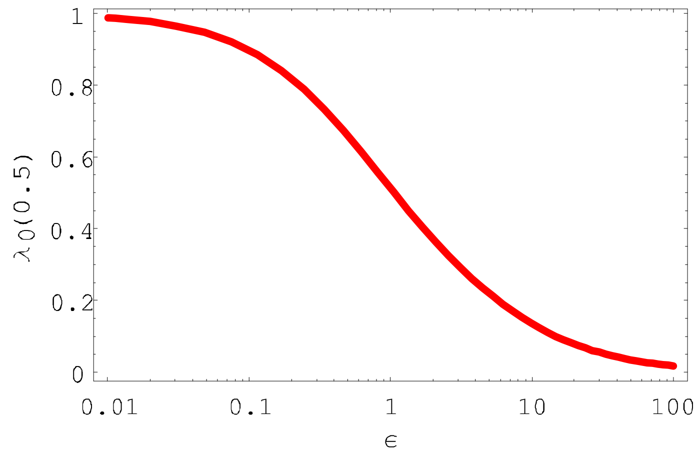


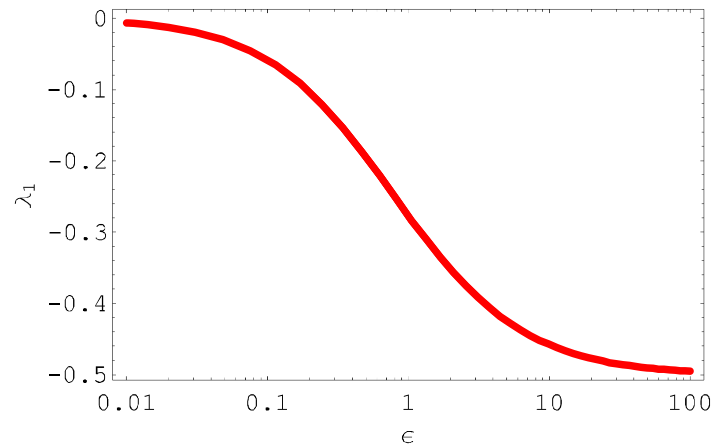


marked linear Knudsen layers, jumps; N must be large $(N \geq 31)$

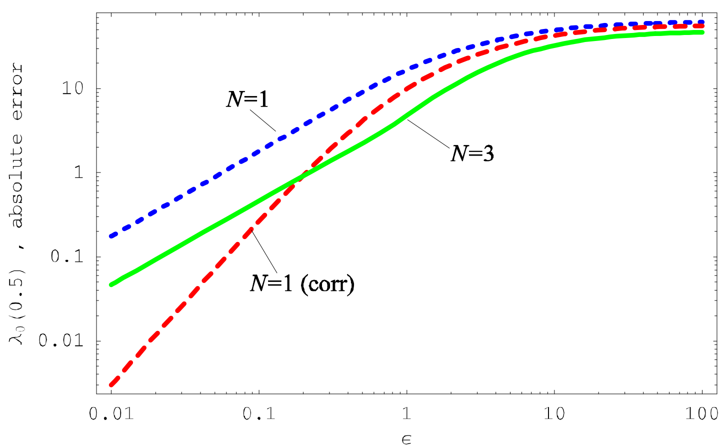
Results for $0 < \varepsilon < \infty$ $(N = 31)$

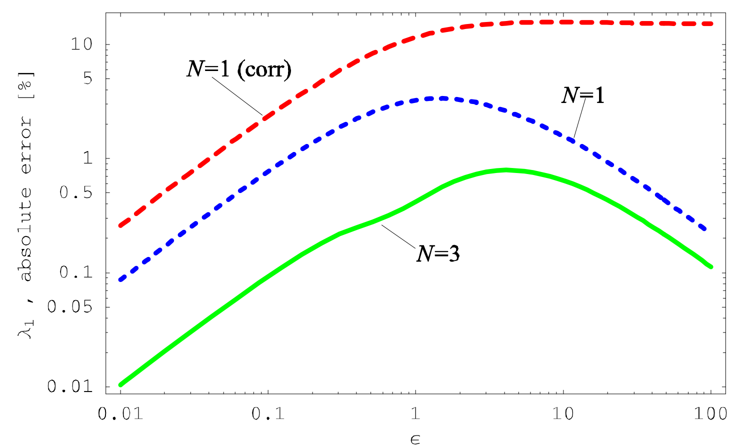
energy density at wall, heat flux





deviation [%] for $N = 1, 3$ [corr: with Knudsen layer correction]

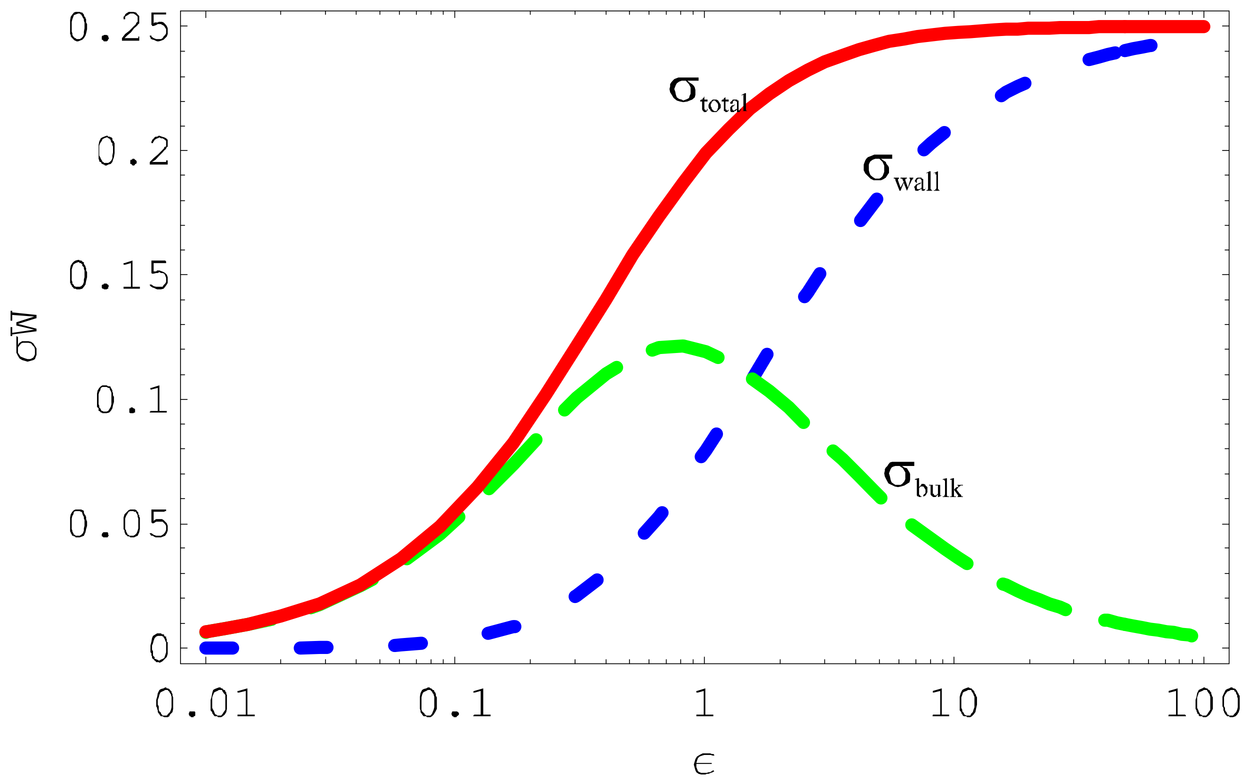




error less than 5% requires $\varepsilon < 0.3$ $(N = 1)$ and $\varepsilon < 1$ $(N = 3)$

Results for $0 < \varepsilon < \infty$ $(N = 31)$

entropy generation: total/bulk/boundary



Asymptotics with boundary conditions

evaluation of bulk eqs and boundary conditions shows

heat flux: $\lambda_1 = \mathcal{O}(\varepsilon)$

energy jump $\bar{\lambda}_0 - \lambda_W = \mathcal{O}(\varepsilon)$

Knudsen layer moments $(n \geq 2)$ $\lambda_n = \mathcal{O}(\varepsilon)$

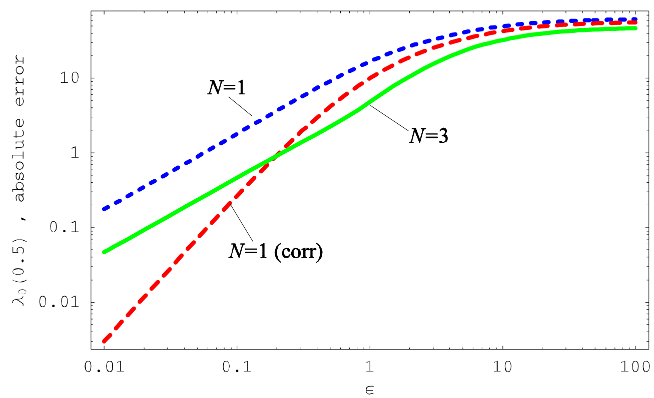
energy first order

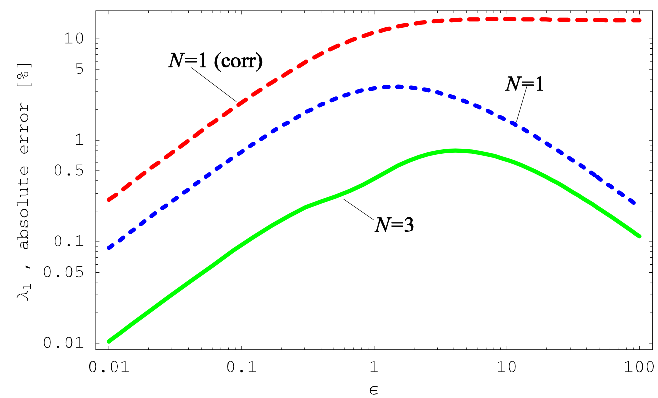
$$\lambda_0 = K - \frac{3}{\varepsilon}\lambda_1 x - 2\lambda_2$$

Knudsen layer correction: assume $\lambda_n \propto \lambda_1$, correction factor ζ of order unity

$$\bar{\lambda}_0 - \lambda_W = -\gamma\frac{2\chi}{2-\chi}\left[\lambda_1 + \sum_{m=2,\ m \text{ even}}^{N} \Psi_{1m}\lambda_m\right] \simeq -\zeta\gamma\frac{2\chi}{2-\chi}\lambda_1$$

improves energy jump, worsens heat flux $\zeta = 0.869$





Asymptotics with boundary conditions

Knudsen layer moments are $\mathcal{O}(\varepsilon)$, contribute to $\mathcal{O}(\varepsilon^2)$

$\Rightarrow$ **higher order theories must include Knudsen layers** of width $\varepsilon b^{(\alpha)}$

$$\Gamma^0_\alpha \exp\left[-\frac{x}{\varepsilon b^{(\alpha)}}\right]$$

N=1:	no Knudsen layer
N=3:	$b^{(a)} = \{\pm 0.5071\}$
N=5	$b^{(l)} = \{\pm 0.8162, \pm 0.3122\}$
N=7:	$b^{(l)} = \{\pm 0.9065, \pm 0.6282, \pm 0.2243\}$

for $\varepsilon < 1$, one (two) Knudsen layer(s) is not too bad $\Longrightarrow$ $N = 3\,(5)$

for $\varepsilon > 1$ need more, criterion presently unclear

$\varepsilon = 1$	$N = 7$
$\varepsilon = 2$	$N = 9$
$\varepsilon = 4$	$N = 11$
$e = 10$	$N = 31$

Conclusions

- linear moment equations with quadratic entropy (H-theorem)
- equivalent to discrete velocity model (DVM)
- boundary conditions from kinetic model
- Knudsen layers (from eigenvalue problem)
- Chapman-Enskog etc valid only in bulk
- Knudsen layers are second order effect
- include at least some Knudsen layers (more is better, but expensive)

Conjecture

- other (linear) moment systems should behave similarly