Singular behavior of a rarefied gas on a planar boundary

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Contents

• Introduction
• Setting of a specific problem
• Macroscopic singularity in physical space
• Microscopic singularity in molecular velocity
• Damping model and the source of macroscopic singularity
• Conclusion
Contents

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• Setting of a specific problem
• Macroscopic singularity in physical space
• Microscopic singularity in molecular velocity
• Damping model and the source of macroscopic singularity
• Conclusion
Introduction
(with a specific example: *thermal transpiration*)

rarefied gas: mean free path $\ell \sim D$

$$k = \frac{\sqrt{\pi}}{2} \frac{\ell}{D}$$: “Knudsen number”
Introduction
(with a specific example: *thermal transpiration*)

rarefied gas: mean free path $\ell \sim D$

$$k = \frac{\sqrt{\pi}}{2} \frac{\ell}{D} : \text{“Knudsen number”}$$
Mass flow ($>0$)

For small $k$ (near continuum limit)
Sone (1969, 2007)
(structure of the Knudsen layer
in the generalized slip-flow theory; BKW or BGK)
For large $k$ (near free molecular limit)
Chen-Liu-T. (preprint)
(math. proof for the hard-sphere gas)

Logarithmic divergence is expected, irrespective of the Knudsen number

cf) Lilly & Sader (2007, 2008)
empirical arguments by a power-law fitting to numerical data

Present concern

$u_2(0)$ vs. $y$:

$u_2(y) - u_2(0) \propto y \ln y$

$\frac{du_2}{dy} \propto \ln y \quad (\rightarrow \infty \quad \text{as} \quad y \rightarrow 0)$

$u_2$ vs. $y$:

$u_2$ vs. $y$
Purpose of research

to confirm

- the same logarithmic gradient divergence occurs irrespective of the Knudsen number

to show

- the above spatial singularity of weighted average of VDF induces another logarithmic gradient divergence in molecular velocity on the boundary

to identify

- the origin of the above singularities, proposing a simple damping model

**Method: analysis + numerics**

These features should be observed generally on a planar boundary, though we deal with only the thermal transpiration here.
Contents

- Introduction
- Setting of a specific problem
- Macroscopic singularity in physical space
- Microscopic singularity in molecular velocity
- Damping model and the source of macroscopic singularity
- Conclusion
Setting of a specific problem
(Thermal transpiration)

Assumptions
- Boltzmann equation (*hard-sphere gas*)
- *diffuse reflection* boundary condition
- $|C| \ll 1$

Then formulate the problem for the perturbation from a local Maxwellian with the wall temperature and the uniform reference pressure
\[
\begin{align*}
\zeta_1 \frac{\partial \phi}{\partial x_1} &= -\frac{1}{k} \nu(|\zeta|) \phi + \frac{1}{k} K[\phi] - \zeta_2(|\zeta|^2 - \frac{5}{2}), \\
b.c. \quad \phi = 0, \quad \zeta_1 \leq 0, \quad x_1 = \pm \frac{1}{2}.
\end{align*}
\]

\(\phi(x_1, \zeta)\): perturbation of VDF (divided by \(C\))

\(\zeta\): dimensionless molecular velocity

\(E(|\zeta|) = \pi^{-3/2} \exp(-|\zeta|^2)\): normalized reference absolute Maxwellian

**Hard-sphere gas**

\[
\nu(|\zeta|) = \frac{1}{2\sqrt{2}} \left( \exp(-|\zeta|^2) + (2|\zeta| + \frac{1}{|\zeta|}) \int_0^{\|\zeta\|} \exp(-t^2) \, dt \right),
\]

\[
K[\Phi] = \int \kappa(\xi, \zeta) \Phi(\xi) E(|\xi|) \, d\xi,
\]

\[
\kappa(\xi, \zeta) = \frac{\sqrt{\pi}}{\sqrt{2}} \frac{1}{|\xi - \zeta|} \exp \left( \frac{|\xi \times \zeta|^2}{|\xi - \zeta|^2} \right) - \frac{\sqrt{\pi}}{2\sqrt{2}} |\xi - \zeta|,
\]
\begin{equation}
\zeta_1 \frac{\partial \phi}{\partial x_1} = -\frac{1}{k} \nu(|\zeta|) \phi + \frac{1}{k} K[\phi] - \zeta_2(|\zeta|^2 - \frac{5}{2}),
\end{equation}

b.c. \quad \phi = 0, \quad \zeta_1 \leq 0, \quad x_1 = \pm \frac{1}{2}.

**NOTE 1**

This problem can be solved formally as

\[ \phi = \int_{\mp 1/2}^{x_1} \frac{1}{k \zeta_1} \exp \left( -\frac{\nu(|\zeta|)}{k |\zeta_1|} |x_1 - s| \right) K[\phi](s, \zeta) ds + \phi_0, \quad \zeta_1 \geq 0, \]

where

\[ \phi_0 = -\frac{k}{\nu(|\zeta|)} [1 - \exp \left( -\frac{\nu(|\zeta|)}{k \zeta_1} (x_1 \pm \frac{1}{2}) \right)] I, \quad \zeta_1 \geq 0, \]

\[ I = \zeta_2(|\zeta|^2 - \frac{5}{2}). \]
\[ \zeta_1 \frac{\partial \phi}{\partial x_1} = -\frac{1}{k} \nu(|\zeta|) \phi + \frac{1}{k} K[\phi] - \zeta_2 (|\zeta|^2 - \frac{5}{2}), \]

b.c. \( \phi = 0, \quad \zeta_1 \ll 0, \quad x_1 = \pm \frac{1}{2}. \)

NOTE 2

\( \phi/\zeta_2 \) can be sought as a function of three variables \((x_1, \zeta_1, |\zeta|)\) or \((x_1, \mu, \zeta)\) by using new coordinates \( \zeta = |\zeta|, \mu = \zeta_1/\zeta, \tan \varphi = \zeta_3/\zeta_2. \)

All the moments of \( \phi \) up to the second order vanish except for the mass flow \( u_2 \) in the \( x_2 \)-direction

\[ u_2[\phi] = \int \zeta_2 \phi E(|\zeta|) d\zeta \]

\[ E(|\zeta|) = \pi^{-3/2} \exp(-|\zeta|^2) \]
Contents

- Introduction
- Setting of a specific problem
- Macroscopic singularity in physical space
- Microscopic singularity in molecular velocity
- Damping model and the source of macroscopic singularity
- Conclusion
Gradient divergence of $u_2$: Basic structure

$$\zeta_1 \frac{\partial \phi}{\partial x_1} = -\frac{1}{k} \nu(|\zeta|) \phi + \frac{1}{k} K[\phi] - \zeta_2 (|\zeta|^2 - \frac{5}{2}),$$

b.c. $\phi = 0$, $\zeta_1 \leq 0$, $x_1 = \pm \frac{1}{2}$.

This problem can be solved formally as

$$\phi = \int_{-1/2}^{x_1} \frac{1}{k\zeta_1} \exp \left( -\frac{\nu(|\zeta|)}{k|\zeta|} |x_1 - s| \right) K[\phi](s, \zeta) ds + \phi_0, \quad \zeta_1 \geq 0,$$

where

$$\phi_0 = -\frac{k}{\nu(|\zeta|)} \left[ 1 - \exp \left( -\frac{\nu(|\zeta|)}{k\zeta_1} (x_1 \pm \frac{1}{2}) \right) \right] I, \quad \zeta_1 \geq 0,$$

$$I = \zeta_2 (|\zeta|^2 - \frac{5}{2}).$$
Gradient divergence of $u_2$: Basic structure

$$
\zeta_1 \frac{\partial \phi}{\partial x_1} = -\frac{1}{k} \nu(\|\zeta\|) \phi + \frac{1}{k} K[\phi] - \zeta_2 (\|\zeta\|^2 - \frac{5}{2}),
$$

b.c. $\phi = 0$, $\zeta_1 \leq 0$, $x_1 = \pm \frac{1}{2}$.

This problem can be solved formally as

$$
\phi = \int_{x_1/2}^{x_1} \frac{1}{k \zeta_1} \exp \left( -\frac{\nu(\|\zeta\|)}{k} |r_1 - s| \right) K[\phi](s, \zeta) \, ds + \phi_0, \quad \zeta_1 \geq 0,
$$

where

$$
\phi_0 = -\frac{k}{\nu(\|\zeta\|)} \left[ 1 - \exp \left( -\frac{\nu(\|\zeta\|)}{k \zeta_1} (x_1 \pm \frac{1}{2}) \right) \right] I, \quad \zeta_1 \geq 0,
$$

$$
I = \zeta_2 (\|\zeta\|^2 - \frac{5}{2}).
$$
\[ u_2[\phi_0] = \int \zeta_2 \phi_0 E \, d\zeta \quad \text{(} x_1 \pm 1/2 \text{) ln}|x_1 \pm 1/2| \]

\[ = \frac{k}{6\sqrt{\pi}} \sum_{i=+, -} \int_0^\infty \frac{\zeta^4}{\nu(\zeta)} (\zeta^2 - \frac{5}{2})(a_i^2 - 6)a_i \text{Ei}(1, a_i) \exp(-\zeta^2) \, d\zeta \]

\[ + \frac{k}{6\sqrt{\pi}} \sum_{i=+, -} \int_0^\infty \frac{\zeta^4}{\nu(\zeta)} (\zeta^2 - \frac{5}{2})(4 + a_i - a_i^2) \exp(-a_i - \zeta^2) \, d\zeta \]

\[ - \frac{4k}{3\sqrt{\pi}} \int_0^\infty \frac{\zeta^4}{\nu(\zeta)} (\zeta^2 - \frac{5}{2}) \exp(-\zeta^2) \, d\zeta, \]

where

\[ a_\pm = \frac{\nu(\zeta)}{k\zeta} |x_1 \pm \frac{1}{2}|, \quad \text{Ei}(1, a > 0) = \int_1^\infty \frac{1}{x} \exp(-ax) \, dx. \]

\[ \text{Ei}(1, a > 0) = -\gamma - \ln a + e^{-a} \sum_{n=1}^\infty \frac{1}{n!} \left( \sum_{r=1}^n \frac{1}{r} \right) a^n, \quad (\gamma: \text{Euler’s constant}), \]
Gradient divergence of $u_2$: Basic structure

$$\zeta_1 \frac{\partial \phi}{\partial x_1} = -\frac{1}{k} \nu(\|\zeta\|) \phi + \frac{1}{k} K[\phi] - \zeta_2 (\|\zeta\|^2 - \frac{5}{2}),$$

b.c. $\phi = 0$, $\zeta_1 \leq 0$, $x_1 = \pm \frac{1}{2}$.

This problem can be solved formally as

$$\phi = \int_{\mp 1/2}^{x_1} \frac{1}{k \zeta_1} \exp \left( -\frac{\nu(\|\zeta\|)}{k \zeta_1} |r_1 - s| \right) K[\phi](s, \zeta_1) ds + \phi_0, \quad \zeta_1 \geq 0,$$

where

$$\phi_0 = -\frac{k}{\nu(\|\zeta\|)} \left[ 1 - \exp \left( -\frac{\nu(\|\zeta\|)}{k \zeta_1} (x_1 \pm \frac{1}{2}) \right) \right] I, \quad \zeta_1 \geq 0,$$

$$I = \zeta_2 (\|\zeta\|^2 - \frac{5}{2}).$$
Gradient divergence of $u_2$: Basic structure

$$\zeta_1 \frac{\partial \phi}{\partial x_1} = -\frac{1}{k} \nu(\|\zeta\|) \phi + \frac{1}{k} \frac{K[\phi]}{\zeta_1} - \zeta_2 \left(\|\zeta\|^2 - \frac{5}{2}\right),$$

b.c. $\phi = 0, \quad \zeta_1 \leq 0, \quad x_1 = \pm\frac{1}{2}$.

This problem can be solved $\phi_0 = \int_{\mp\frac{1}{2}}^{x_1} \frac{1}{\zeta_1} \exp \left(-\frac{\nu}{k\|\zeta_1\|} |x_1 - s| \right) I ds$

$$\phi = \int_{\mp\frac{1}{2}}^{x_1} \frac{1}{k\zeta_1} \exp \left(-\frac{\nu(\|\zeta\|)}{k\|\zeta_1\|} |x_1 - s| \right) K[\phi](s,\zeta) ds + \phi_0, \quad \zeta_1 \geq 0,$$

where

$$\phi_0 = -\frac{k}{\nu(\|\zeta\|)} [1 - \exp \left(-\frac{\nu(\|\zeta\|)}{k\zeta_1} (x_1 \pm \frac{1}{2}) \right)] I, \quad \zeta_1 \geq 0,$$

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Gradient divergence of $u_2$: Basic structure

$$\zeta_1 \frac{\partial \phi}{\partial x_1} = -\frac{1}{k} \nu(|\zeta|) \phi + \frac{1}{k} K[\phi] - \zeta_2 (|\zeta|^2 - \frac{5}{2}),$$

b.c. $\phi = 0, \; \zeta_1 \equiv 0, \; x_1 = \pm \frac{1}{2}$.

This problem can be solved

$$\phi_0 = \int_{\mp \frac{1}{2}}^{x_1} \frac{1}{\zeta_1} \exp \left(-\frac{\nu}{k|\zeta_1|} |x_1 - s| \right) I ds$$

$$\phi = \int_{\mp \frac{1}{2}}^{x_1} \frac{1}{k\zeta_1} \exp \left(-\frac{\nu(|\zeta|)}{k|\zeta_1|} |x_1 - s| \right) K[\phi](s, \zeta) ds + \phi_0, \; \zeta_1 \geqslant 0,$$

where

$$\phi_0 = -\frac{k}{\nu(|\zeta|)} \left[1 - \exp \left(-\frac{\nu(|\zeta|)}{k|\zeta_1|} (x_1 \pm \frac{1}{2}) \right) \right] I, \; \zeta_1 \geqslant 0,$$

$$I = \zeta_2 (|\zeta|^2 - \frac{5}{2}).$$
Gradient divergence of $u_2$: Basic structure

$$\zeta_1 \frac{\partial \phi}{\partial x_1} = -\frac{1}{k} \nu(|\zeta|) \phi + \frac{1}{k} K[\phi] - \zeta_2 (|\zeta|^2 - \frac{5}{2}).$$

b.c. $\phi = 0, \quad \zeta_1 \leq 0, \quad x_1 = \pm \frac{1}{2}$.

This problem can be solved if

$$\phi_0 = \int_{\mp \frac{1}{2}}^{x_1} \frac{1}{\zeta_1} \exp \left( -\frac{\nu}{k|\zeta_1|} |x_1 - s| \right) I ds$$

$$\phi = \int_{\mp \frac{1}{2}}^{x_1} \frac{1}{k \zeta_1} \exp \left( -\frac{\nu(|\zeta|)}{k|\zeta_1|} |x_1 - s| \right) K[\phi](s, \zeta) ds + \phi_0, \quad \zeta_1 \geq 0,$$

where

$$\phi_0 = -\frac{k}{\nu(|\zeta|)} \left[ 1 - \exp \left( -\frac{\nu(|\zeta|)}{k|\zeta_1|} (x_1 \pm \frac{1}{2}) \right) \right] I, \quad \zeta_1 \geq 0,$$

$$I = \zeta_2 (|\zeta|^2 - \frac{5}{2}).$$

Since the structure is the same, the same singular nature is expected from the $K$ part (as far as the $K$ behaves well).
Mass flow profile near the boundary

- $u_2$ (Mass flow) $> 0$

- $k = 10$
- $k = 6$
- $k = 2$
- $k = 1$
- $k = 0.6$

Heat flow

- Open circle: present numerical result
- Solid line: least mean square approx.

$$a + b(1/2 - x_1) \ln(1/2 - x_1) + c(1/2 - x_1)$$
Mass flow profile near the boundary

Mass flow ( > 0)

open circle: present numerical result
solid line: least mean square approx.

\[ a + b(1/2 - x_1) \ln(1/2 - x_1) + c(1/2 - x_1) \]
Contents

• Introduction
• Setting of a specific problem
• Macroscopic singularity in physical space
• Microscopic singularity in molecular velocity
• Damping model and the source of macroscopic singularity
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Velocity distribution function on the boundary for $|\zeta| = 1$

- (a) $k = 6$
- (b) $k = 1$
- (c) $k = 0.6$

Common feature for impinging molecules to the boundary, almost parallel to it.
At $x_1 = 1/2$

$$
\phi = \begin{cases} 
\int_{-1/2}^{1/2} \frac{1}{k \zeta_1} \exp \left( -\frac{\nu}{k \zeta_1} \left( \frac{1}{2} - s \right) \right) K[\phi](s, \zeta) ds + \phi_0, & \zeta_1 > 0, \\
0, & \zeta_1 < 0.
\end{cases}
$$

$$
\phi_0 = -(k/\nu)[1 - \exp (-\nu/k \zeta_1)] I \text{ for } \zeta_1 > 0,
$$

BGK (or BKW) model: \( K[\phi] = 2\zeta_2 u_2[\phi] \)

\( K[\phi](s) \) is singular in \( s \) at \( s = \pm \frac{1}{2} \) as \((s \mp \frac{1}{2}) \ln |s \mp \frac{1}{2}|\)

because of \( u_2[\phi](s) \) but is regular in \(|\zeta|\)

We expect the same property for the Boltzmann collision kernel
Evidence \[ K[\phi](s = \frac{1}{2}, \zeta) \] on the boundary

(a) \( k = 6 \)  
(b) \( k = 1 \)  
(c) \( k = 0.6 \)

\[
K[\phi] = (\zeta_2 / |\zeta|) [ f_-(\zeta_1, |\zeta|)(s - \frac{1}{2}) \ln |s - \frac{1}{2}| + f_+(\zeta_1, |\zeta|)(s + \frac{1}{2}) \ln (s + \frac{1}{2}) \\
+ f_0(\zeta_1, |\zeta|) + \sum_{m=1}^{\infty} s^m f_m(\zeta_1, |\zeta|) ].
\]
At $x_1 = 1/2$

$$
\phi = \begin{cases} 
\int_{-1/2}^{1/2} \frac{1}{k \zeta_1} \exp \left( -\frac{\nu}{k \zeta_1} \left( \frac{1}{2} - s \right) \right) K[\phi](s, \zeta) \, ds + \phi_0, & \zeta_1 > 0, \\
0, & \zeta_1 < 0.
\end{cases}
$$

\[
K[\phi] = (\zeta_2 / |\zeta|) \left[ f_-(\zeta_1, |\zeta|)(s - \frac{1}{2}) \ln |s - \frac{1}{2}| + f_+(\zeta_1, |\zeta|)(s + \frac{1}{2}) \ln (s + \frac{1}{2}) \right] 
+ f_0(\zeta_1, |\zeta|) + \sum_{m=1}^{\infty} s^m f_m(\zeta_1, |\zeta|).
\]

$\phi \sim \zeta_1 \ln \zeta_1$ for small $\zeta_1 > 0$ and thus its gradient diverges logarithmically as $\zeta_1 \to 0_+$. 
Numerical validation

\[ \phi = \int_{-1/2}^{x_1} \frac{1}{k|\zeta_1|} \exp \left( -\frac{\nu(|\zeta|)}{k^2|\zeta_1|} |x_1 - s| \right) K[\phi](s, \zeta) ds + \phi_0, \quad \zeta_1 \geq 0, \]

Two methods have been tested for numerical integration

**Method 1. Piecewise quadratic interpolation in s**

**Method 2. Piecewise quadratic + \( s \ln s \) interpolation in s**

for \( K[\phi] \) from its discretized data

\[ K[\phi] = (\zeta_2/|\zeta|)[f_- (\zeta_1, |\zeta|)(s - \frac{1}{2}) \ln |s - \frac{1}{2}| + f_+ (\zeta_1, |\zeta|)(s + \frac{1}{2}) \ln (s + \frac{1}{2}) + f_0 (\zeta_1, |\zeta|) + \sum_{m=1}^{\infty} s^m f_m (\zeta_1, |\zeta|)]. \]

This part is missing in Method 1
**Evidence**

Velocity distribution func. on the boundary

(a) $k = 6$

(b) $k = 1$

(c) $k = 0.6$

\[ x_1 = \frac{1}{2}, \ |\zeta| = 0.5 \]

<table>
<thead>
<tr>
<th>Method</th>
<th>Grid</th>
<th>Note</th>
</tr>
</thead>
<tbody>
<tr>
<td>Method 1</td>
<td>C1</td>
<td>I1, F1</td>
</tr>
<tr>
<td></td>
<td></td>
<td>Slow convergence</td>
</tr>
<tr>
<td>Method 2</td>
<td>C2</td>
<td>F2</td>
</tr>
<tr>
<td></td>
<td></td>
<td>Satisfactory convergence</td>
</tr>
</tbody>
</table>

Validate the logarithmic singularity of VDF on the boundary
Contents

- Introduction
- Setting of a specific problem
- Macroscopic singularity in physical space
- Microscopic singularity in molecular velocity
- Damping model and the source of macroscopic singularity
- Conclusion
Contribution to macroscopic singularity

\[ \phi = \int_{x_1}^{x_1} \frac{1}{k\zeta_1} \exp \left( -\frac{\nu(|\zeta|)}{k|\zeta_1|} |x_1 - s| \right) K[\phi](s, \zeta) ds + \phi_0, \quad \zeta_1 \geq 0, \]

\[ K[\phi] = (\zeta_2/|\zeta|)[f_-(\zeta_1, |\zeta|)(s - \frac{1}{2}) \ln |s - \frac{1}{2}| + f_+(\zeta_1, |\zeta|)(s + \frac{1}{2}) \ln(s + \frac{1}{2})
\]

\[ + f_0(\zeta_1, |\zeta|) + \sum_{m=1}^{\infty} s^m f_m(\zeta_1, |\zeta|). \]

1. No contribution from \( \zeta_1 > 0 \) (impinging side)
2. Contribution only from \( f_0(\zeta_1 = 0, |\zeta|) \) for \( \zeta_1 < 0 \) (reflected side)

\[ \Rightarrow \text{same as the contribution from} \]

\[ \phi_0 = \int_{x_1}^{-1/2} \frac{1}{\zeta_1} \exp \left( -\frac{\nu}{k|\zeta_1|} |x_1 - s| \right) I ds. \]
Keeping in mind the item 2 in the previous slide, we define

\[
f := \int_{\pm \frac{1}{2}}^{x_1} \frac{1}{k \zeta_1} \exp \left( -\frac{\nu}{k|\zeta_1|} |x_1 - s| \right) I ds \\
+ \int_{\pm \frac{1}{2}}^{x_1} \frac{1}{k \zeta_1} \exp \left( -\frac{\nu}{k|\zeta_1|} |x_1 - s| \right) \frac{1}{k} K[\phi]|_{\zeta_1=0, x_1=\pm \frac{1}{2}} ds, \quad \zeta_1 \leq 0
\]

Note: \( \phi = \int_{\pm 1/2}^{x_1} \frac{1}{k \zeta_1} \exp \left( -\frac{\nu(|\zeta|)}{k|\zeta_1|} |x_1 - s| \right) K[\phi](s, \zeta) ds + \phi_0, \quad \zeta_1 \geq 0. \)

\[
f = -\frac{k}{\nu} \left( \frac{1}{k} K[\phi] - I \right)|_{\zeta_1=0, x_1=\pm 1/2} \exp \left( -\frac{\nu}{k \zeta_1} \left( x_1 + \frac{1}{2} \right) \right), \quad \zeta_1 \leq 0. \quad (5.1)
\]

The singularity of \( u_2[\phi] \) should be reproduced by the corresponding moment \( u_2[f] \) of \( f \)

Equation (5.1) is the solution of a simple damping model

\[
\zeta_1 \frac{\partial f}{\partial x_1} = -\frac{\nu}{k} f, \quad (5.2a)
\]

\[
f = -\frac{k}{\nu} \left( \frac{1}{k} K[\phi] - I \right)|_{\zeta_1=0, x_1=\pm 1/2}, \quad \zeta_1 \leq 0, \quad x_1 = \pm 1/2. \quad (5.2b)
\]
Keeping in mind the item 2 in the previous slide, we define

\[ f := \int_{\mp \frac{1}{2}}^{x_1} \frac{1}{\zeta_1} \exp \left( -\frac{\nu}{k|\zeta_1|} |x_1 - s| \right) I ds + \int_{\mp \frac{1}{2}}^{x_1} \frac{1}{k\zeta_1} \exp \left( -\frac{\nu}{k|\zeta_1|} |x_1 - s| \right) \frac{1}{k} K[\phi]|_{\zeta_1=0, x_1=\pm \frac{1}{2}} ds, \quad \zeta_1 \leq 0 \]

**Note:** \( \phi = \int_{\mp 1/2}^{x_1} \frac{1}{k\zeta_1} \exp \left( -\frac{\nu(|\zeta|)}{k|\zeta_1|} |x_1 - s| \right) K[\phi](s, \zeta) ds + \phi_0, \quad \zeta_1 \geq 0 \).

\[ f = -\frac{k}{\nu} \left( \frac{1}{k} K[\phi] - I \right)|_{\zeta_1=0, x_1=\pm 1/2} \exp \left( -\frac{\nu}{k\zeta_1} (x_1 + \frac{1}{2}) \right), \quad \zeta_1 \leq 0. \quad (5.1) \]

The singularity of \( u_2[\phi] \) should be reproduced by the corresponding moment \( u_2[f] \) of \( f \).

Equation (5.1) is the solution of a simple damping model

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Keeping in mind the item 2 in the previous slide, we define

\[ f := \int_{\mp \frac{1}{2}}^{x_1} \frac{1}{\zeta_1} \exp \left( -\frac{\nu}{k|\zeta_1|} |x_1 - s| \right) I ds \]

\[ + \int_{\mp \frac{1}{2}}^{x_1} \frac{1}{k\zeta_1} \exp \left( -\frac{\nu}{k|\zeta_1|} |x_1 - s| \right) \frac{1}{k} K[\phi]|_{\zeta_1=0, x_1=\pm \frac{1}{2}} ds, \quad \zeta_1 \leq 0 \]

\[ \phi = \int_{\mp 1/2}^{x_1} \frac{1}{k\zeta_1} \exp \left( -\frac{\nu(|\zeta_1|)}{k|\zeta_1|} |x_1 - s| \right) K[\phi](s, \zeta) ds + \phi_0, \quad \zeta_1 \geq 0. \]

\[ f = -\frac{k}{\nu} \left( \frac{1}{k} K[\phi] - I \right)|_{\zeta_1=0, x_1=\pm 1/2} \exp \left( -\frac{\nu}{k\zeta_1} (x_1 + \frac{1}{2}) \right), \quad \zeta_1 \leq 0. \quad (5.1) \]

The singularity of \( u_2[\phi] \) should be reproduced by the corresponding moment \( u_2[f] \) of \( f \)

Equation (5.1) is the solution of a simple damping model

\[ \zeta_1 \frac{\partial f}{\partial x_1} = -\frac{\nu}{k} f, \quad (5.2a) \]

\[ f = -\frac{k}{\nu} \left( \frac{1}{k} K[\phi] - I \right)|_{\zeta_1=0, x_1=\pm 1/2}, \quad \zeta_1 \leq 0, x_1 = \pm 1/2. \quad (5.2b) \]
Keeping in mind the item 2 in the previous slide, we define

\[
 f := \int_{x_1}^{x_1} \frac{1}{\zeta_1} \exp \left( - \frac{\nu}{k|\zeta_1|} |x_1 - s| \right) I \, ds \\
+ \int_{x_1}^{x_1} \frac{1}{k\zeta_1} \exp \left( - \frac{\nu}{k|\zeta_1|} |x_1 - s| \right) \frac{1}{k} K[\phi]|_{\zeta_1=0, x_1=\pm \frac{1}{2}} \, ds, \quad \zeta_1 \leq 0
\]

Note: \( \phi = \int_{x_1}^{x_1} \frac{1}{k\zeta_1} \exp \left( - \frac{\nu(|\zeta|)}{k|\zeta_1|} |x_1 - s| \right) K[\phi](s, \zeta) \, ds + \phi_0, \quad \zeta_1 \geq 0. \)

\[
 f = -\frac{k}{\nu} \left( \frac{1}{k} K[\phi] - I \right)|_{\zeta_1=0, x_1=\pm \frac{1}{2}} \exp \left( - \frac{\nu}{k\zeta_1} (x_1 + \frac{1}{2}) \right), \quad \zeta_1 \leq 0. \quad (5.1)
\]

Note: The singularity of \( u_2[\phi] \) should be reproduced by the corresponding moment \( u_2[f] \) of \( f \)

Equation (5.1) is the solution of a simple damping model

\[
 \zeta_1 \frac{\partial f}{\partial x_1} = -\frac{\nu}{k} f, \quad (5.2a)
\]
\[
f = -\frac{k}{\nu} \left( \frac{1}{k} K[\phi] - I \right)|_{\zeta_1=0, x_1=\pm \frac{1}{2}}, \quad \zeta_1 \leq 0, \ x_1 = \pm \frac{1}{2}. \quad (5.2b)
\]
Keeping in mind the item 2 in the previous slide, we define

\[
f := \int_{\mp \frac{1}{2}}^{x_1} \frac{1}{\zeta_1} \exp \left( -\frac{\nu}{k|\zeta_1|} |x_1 - s| \right) I \, ds \\
+ \int_{\mp \frac{1}{2}}^{x_1} \frac{1}{k\zeta_1} \exp \left( -\frac{\nu}{k|\zeta_1|} |x_1 - s| \right) \frac{1}{k} K[\phi]_{\zeta_1=0, x_1=\pm \frac{1}{2}} \, ds, \quad \zeta_1 \leq 0
\]

**Note:** \( \phi = \int_{\mp \frac{1}{2}}^{x_1} \frac{1}{k\zeta_1} \exp \left( -\frac{\nu(|\zeta|)}{k|\zeta|} |x_1 - s| \right) K[\phi](s, \zeta) ds + \phi_0, \quad \zeta_1 \geq 0. \)

\[
f = -\frac{k}{\nu} \left( \frac{1}{k} K[\phi] - I \right)_{\zeta_1=0, x_1=\pm 1/2} \exp \left( -\frac{\nu}{k\zeta_1} (x_1 + \frac{1}{2}) \right), \quad \zeta_1 \leq 0. \quad (5.1)
\]

**Note:** The singularity of \( u_2[\phi] \) should be reproduced by the corresponding moment \( u_2[f] \) of \( f \)

Equation (5.1) is the solution of a simple damping model

\[
\zeta_1 \frac{\partial f}{\partial x_1} = -\frac{\nu}{k} f, \quad \text{What does it mean physically?} \quad (5.2a)
\]

\[
f = -\frac{k}{\nu} \left( \frac{1}{k} K[\phi] - I \right)_{\zeta_1=0, x_1=\pm 1/2}, \quad \zeta_1 \leq 0, \ x_1 = \pm 1/2. \quad (5.2b)
\]
What is it?

\[
f = -\frac{k}{\nu} \left( \frac{1}{k} K[\phi] - I \right) |_{\zeta_1=0, \, x_1=\pm 1/2}, \quad \zeta_1 \leq 0, \, x_1 = \pm 1/2.
\]

Let us go back to the original problem...

\[
\zeta_1 \frac{\partial \phi}{\partial x_1} = -\frac{1}{k} \nu (|\zeta|) \phi + \frac{1}{k} K[\phi] - \zeta_2 (|\zeta|^2 - \frac{5}{2}),
\]

b.c. \( \phi = 0, \quad \zeta_1 \leq 0, \, x_1 = \pm \frac{1}{2}. \) \hspace{1cm} (2.3a)

Since \( \phi \) is a solution of (2.3a), we have

\[
\phi(x_1, \zeta_1 = 0) = \frac{k}{\nu} \left( \frac{1}{k} K[\phi] - I \right) |_{\zeta_1=0} \quad \text{for} \quad -1/2 < x_1 < 1/2.
\]

This expression gives the limiting value of \( \phi \) for \( \zeta_1 = 0_\pm \) and \( x_1 \rightarrow \pm 1/2 \), and thus we have the following relation on the boundary

\[
-\frac{k}{\nu} \left( \frac{1}{k} K[\phi] - I \right) |_{\zeta_1=0, \, x_1=\pm 1/2} = \phi(x_1 = \pm 1/2, \zeta_1 = 0_\mp) - \phi(x_1 = \pm 1/2, \zeta_1 = 0_\pm).
\]

**Origin of the spatial singularity**

**Impinging side limit**

[note: reflected side = 0]
Equation (5.1) is the solution of a simple damping model

\[ \zeta_1 \frac{\partial f}{\partial x_1} = -\frac{\nu}{k} f, \]  
\[ f = -\frac{k}{\nu} \left( \frac{1}{k} K[\phi] - I \right)_{\zeta_1 = 0, x_1 = \pm 1/2}, \quad \zeta_1 \leq 0, \ x_1 = \pm 1/2. \]  

Discontinuity of VDF on the boundary at \( \zeta_1 = 0 \)

(a) \( k = 6 \) 
(b) \( k = 1 \) 
(c) \( k = 0.6 \)

Spatial singularity \((x_1 \pm \frac{1}{2}) \ln |x_1 \pm \frac{1}{2}| \) of \( u_2[\phi] \) is the trace of the discontinuity of \( \phi \) on the boundary at \( \zeta_1 = 0 \). It is produced by the damping of discontinuity through the collision frequency \( \nu \).
Comparison of the coefficient $b$ of $x \ln x$

Original problem vs. Dumping model

\[ a + b(1/2 - x_1) \ln(1/2 - x_1) + c(1/2 - x_1) \]

<table>
<thead>
<tr>
<th>$k$</th>
<th>$u_2[\phi]$</th>
<th>$u_2[f]$</th>
</tr>
</thead>
<tbody>
<tr>
<td>10</td>
<td>-0.1640</td>
<td>-0.1641</td>
</tr>
<tr>
<td>6</td>
<td>-0.1728</td>
<td>-0.1730</td>
</tr>
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<td>1</td>
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<tr>
<td>0.6</td>
<td>-0.2378</td>
<td>-0.2379</td>
</tr>
</tbody>
</table>

Numerically validated
Conclusion

- The logarithmic gradient divergence of macroscopic quantity is confirmed *irrespective of the Knudsen number*.

- The spatial singularity of weighted average of VDF induces *another logarithmic gradient divergence in molecular velocity* on the boundary.

- The origin of the above singularities are *the discontinuity of VDF on the boundary* and can be expressed by its *damping through the collision frequency*. 
Conclusion (# comments)

Our argument applies to

• Cut-off potential models, for which the splitting of the collision integral can be made

• More general boundary condition such as the Maxwell boundary condition (specular+diffuse) and other non-diffuse conditions