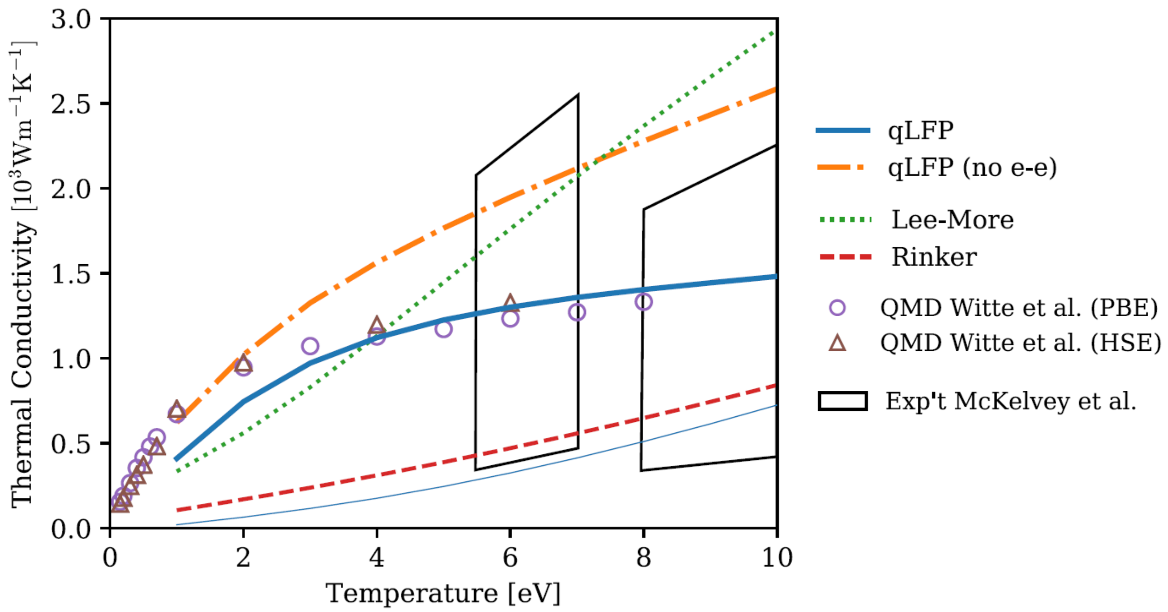
Electron-electron scattering in dense plasma transport: why it matters, why it is difficult, and what we can do about it today



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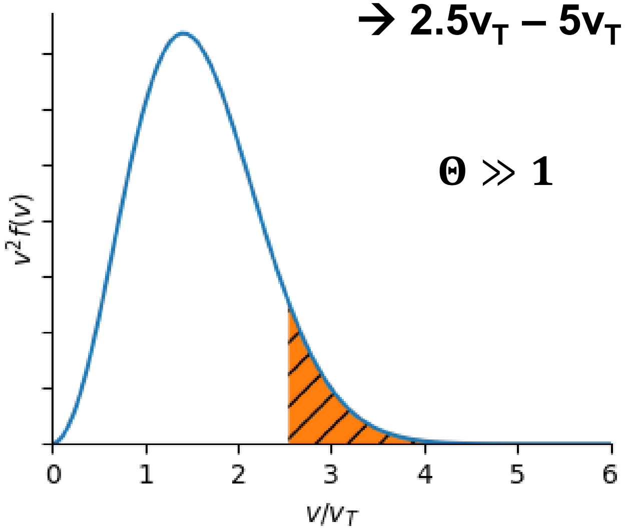
Summary

Accounting for electron-electron scattering is the next theoretical threshold for dense plasma transport calculations to cross

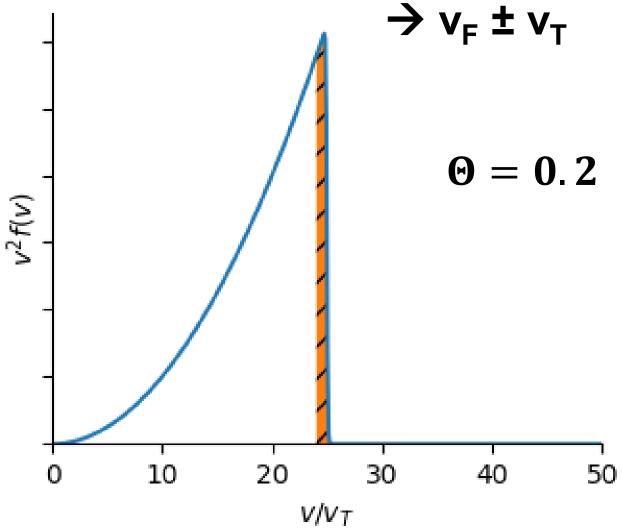
- Why does it matter?
  - Electron-electron scattering is an efficient means of energy transfer between electrons
  - Conduction electron populations are sensitive to e-e scattering
- Why is it difficult?
  - "Ab initio" DFT+KG misses e-e scattering
  - Existing methods for going beyond DFT+KG is very painful (e.g., MBPT)
  - Quantum kinetic theory is not straightforward to evaluate (esp. at strong coupling) and is sensitive to model choices (bound vs free electrons, Coulomb logs)
- What can we do about it today?
  - Quantum Landau/Fokker-Planck kinetic theory with mean-force Coulomb logarithms
  - TD-DFT to quantify dynamic screening of fast electrons relevant to nonlocal conduction

The physics of conduction electrons is highly sensitive to degeneracy

Classical: "conduction"
→ $2.5v_T - 5v_T$



Degenerate: "conduction"
→ $v_F \pm v_T$

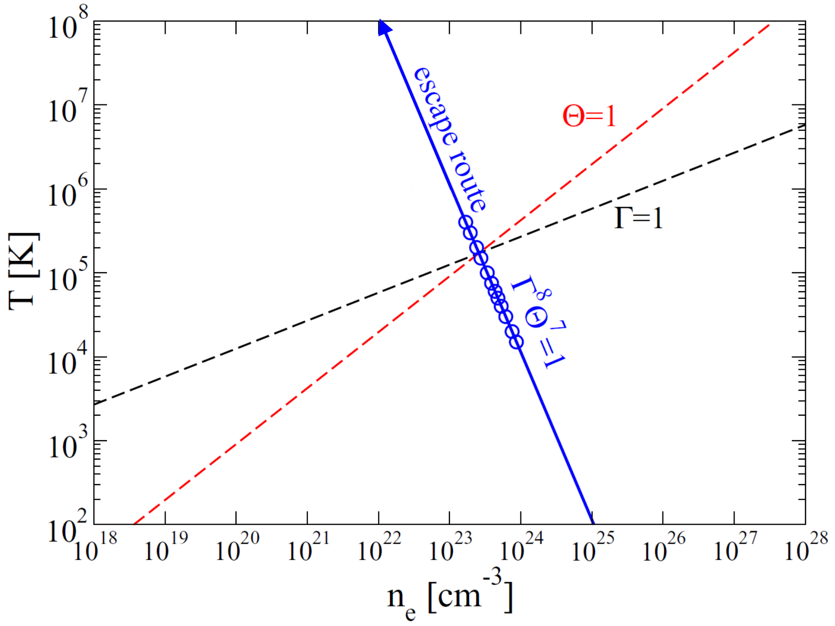


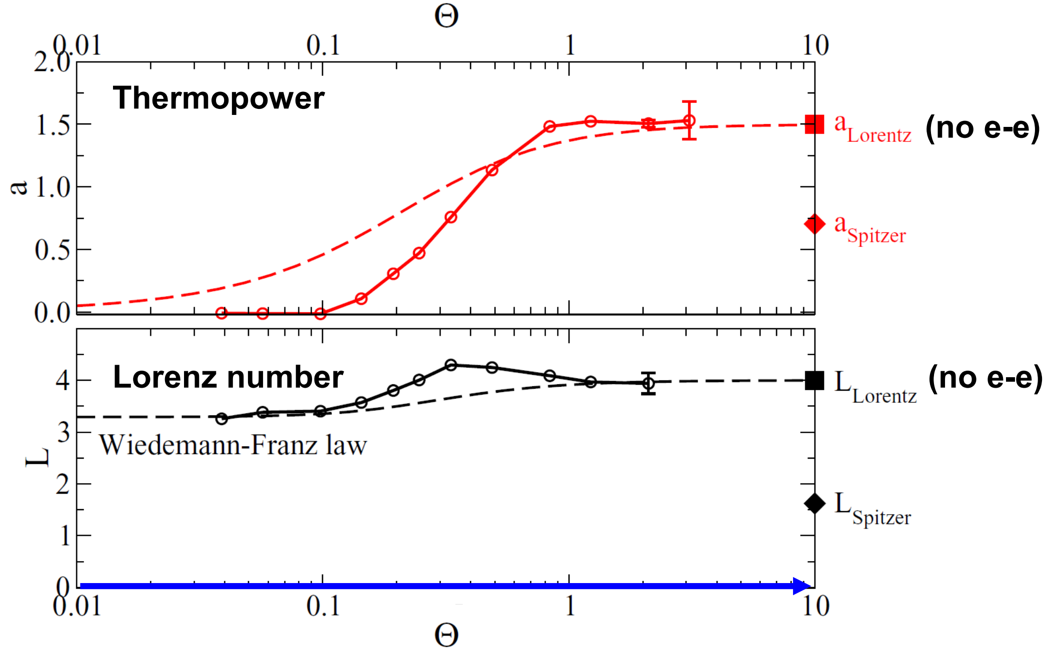
(hydrogen*,**) $\frac{\sigma(\text{with ee})}{\sigma(\text{no ee})} \sim 2$ $\frac{\kappa(\text{with ee})}{\kappa(\text{no ee})} \sim 4$ $\frac{\sigma(\text{with ee})}{\sigma(\text{no ee})} \sim 1$ $\frac{\kappa(\text{with ee})}{\kappa(\text{no ee})} \sim 1?$

How quickly is the degenerate limit reached?

* L. Spitzer, Jr. and R. Härm, *Phys. Rev.* 89, 977 (1953).
** H. Reinholz et al., *Phys. Rev. E* 91, 043105 (2015).

The latest Kubo-Greenwood calculations approaching the non-degenerate limit show a total absence of electron-electron scattering

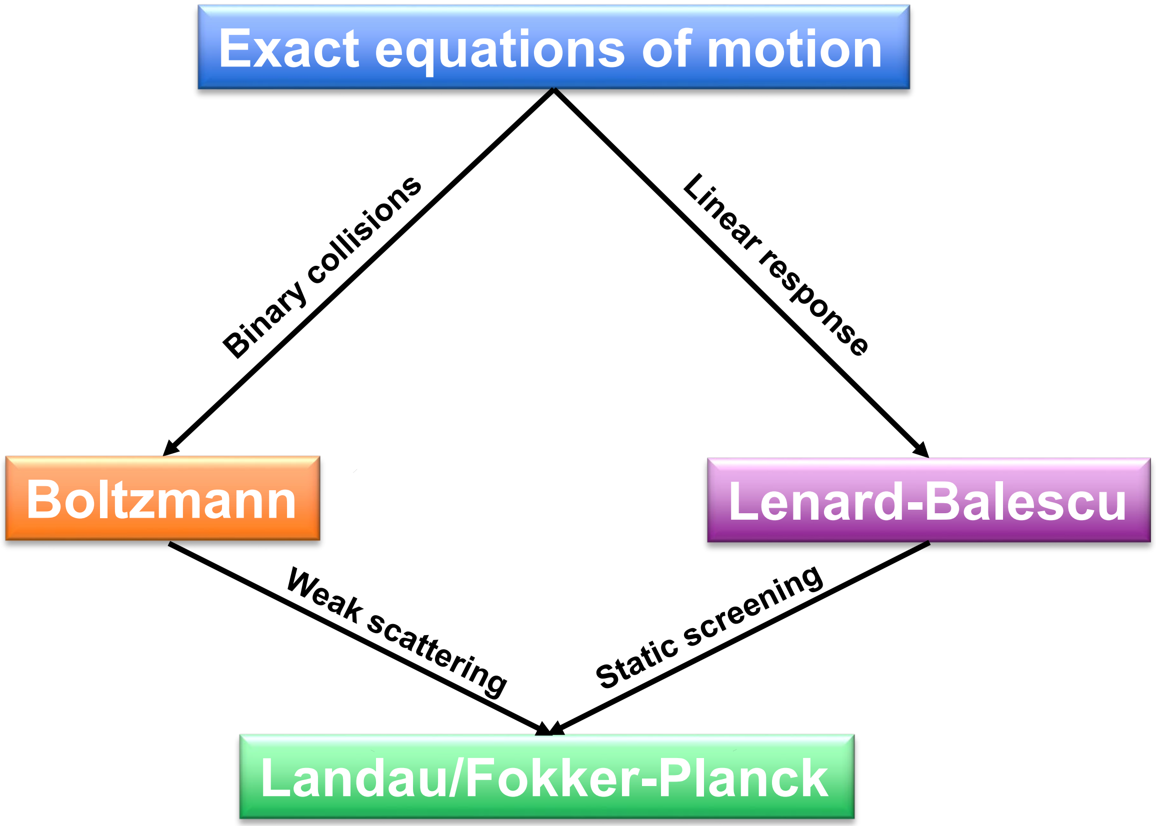




Until we have "ab initio" methods that include e-e scattering, there is no theoretical gold standard to judge simpler models

* M. French et al., *Phys. Rev. E* 105, 065204 (2022).

In the absence of a high-fidelity simulation method, our best available tool is quantum kinetic theory



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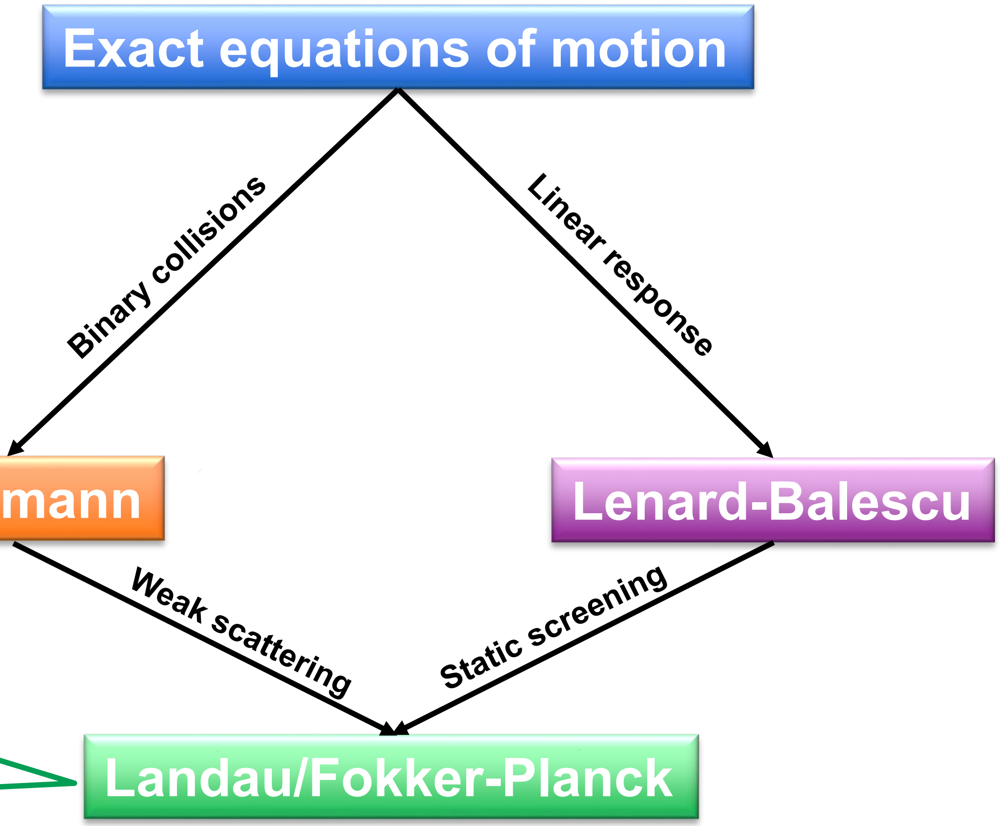


Key quantity: Coulomb logarithm

Solutions known at any degeneracy

“Solution” == “Champan-Enskog solution”

* J. Daligault, *Phys. Plasmas* 25, 082703 (2018).

A quantum Landau/Fokker-Planck model is a practical way to extend non-degenerate plasma kinetic theory to moderate degeneracy

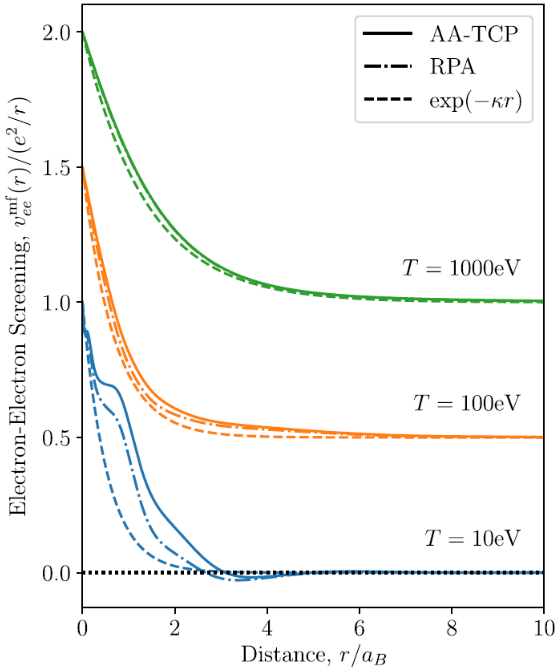
- Coulomb logarithms are a convenient entry point for patching in strong-coupling effects
- Construct from mean-force scattering cross-sections, $\sigma_{ei}(E)$ and $\sigma_{ee}(E)$

$$\sigma_{ei}^{(1)}(E) = \frac{4\pi}{k^2}\sum_{l=0}^{\infty}(l+1)\sin^2(\delta_{l+1}-\delta_l)$$

$$\sigma_{ee}^{(2)}(E) = \frac{4\pi}{k^2}\sum_{l=0}^{\infty}\frac{(l+1)(l+2)}{2l+3}\sin^2(\delta_{l+2}-\delta_l)\left[1-\frac{1}{2}(-1)^l\right]$$

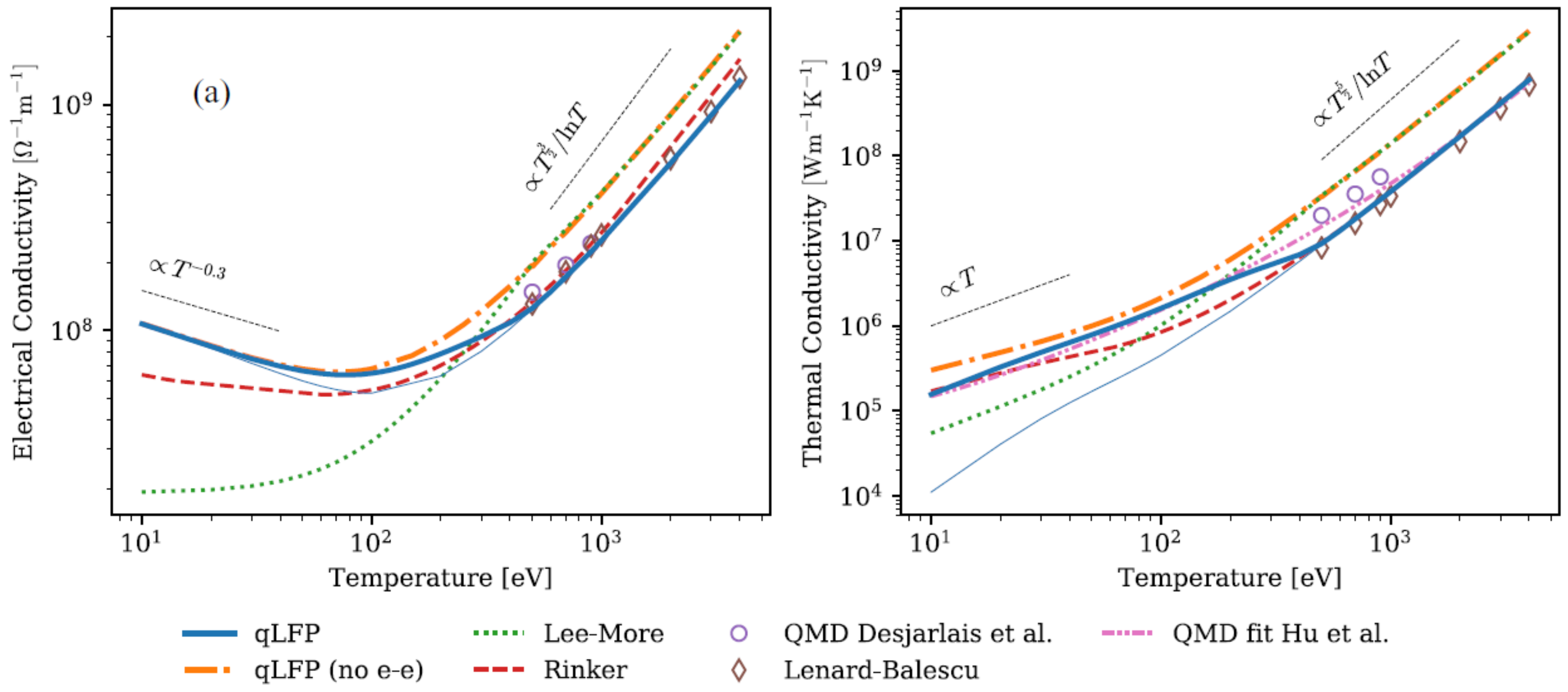
Electron indistinguishability

- Mean-force potentials provided by average-atom two-component plasma model
  - Recovers Debye-Hückel/Thomas-Fermi screening in ideal limit
  - Accounts for static correlations at non-ideal conditions
  - Includes effects of ion shell structure at short range



* J. Daligault, *Phys. Plasmas* 25, 082703 (2018).
** C. E. Starrett, *High Energy Density Phys.* 25, 8 (2017).
† N. R. Shaffer & C. E. Starrett, *Phys. Rev. E* 101, 013208 (2020).
‡ N. R. Shaffer and C. E. Starrett, *Phys. Rev. E* 101, 052304 (2020).

Transport calculations in hydrogen highlight the importance of e-e scattering in the non-degenerate and partially degenerate regimes

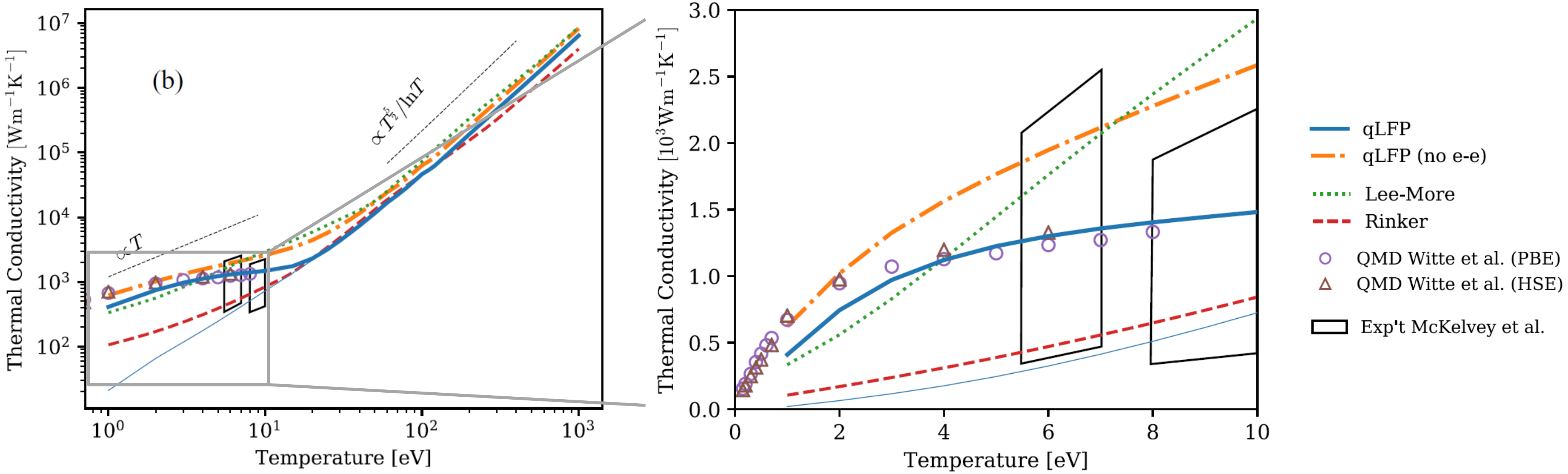


Quantum kinetic theories agree for weakly degenerate plasmas, but low-temperature behavior is less clear.

Hydrogen
$\rho = 40 \text{ g/cm}^3$

* N. R. Shaffer and C. E. Starrett, *Phys. Rev. E* 101, 052304 (2020).
** Y. T. Lee and R. M. More, *Phys. Fluids* 27, 1273 (1984).
† M. P. Desjarlais et al., *Phys. Rev. E* 95, 033203 (2017).
‡ S. X. Hu et al., *Phys. Rev. E* 89, 043105 (2014).

QMD results and experimental measurements of solid-density Al benchmark qLFP's behavior at low temperatures



qLFP predicts e-e collisions remain relevant at low temperatures, but more sophisticated theories are needed.

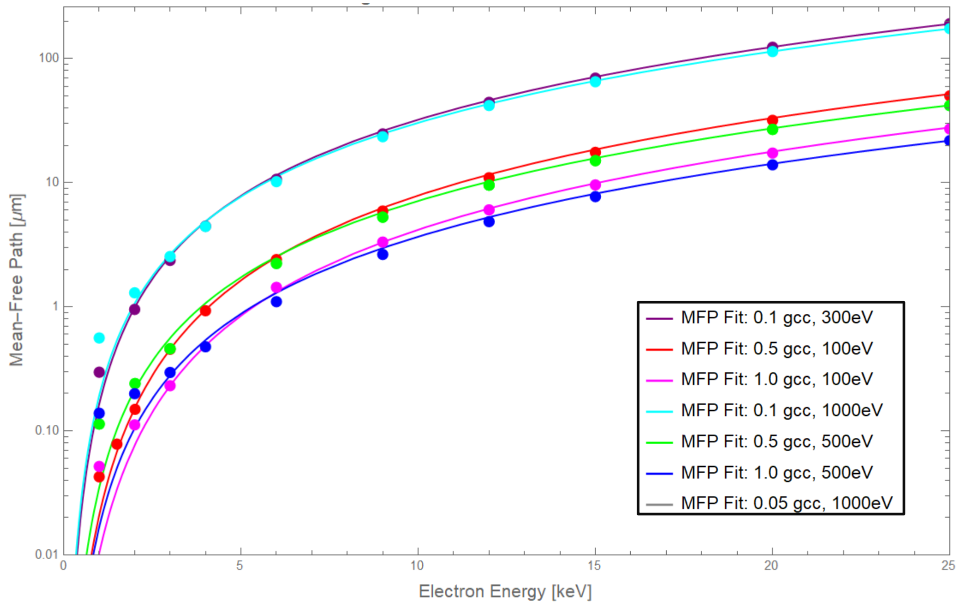
Aluminum
$\rho = 2.7\ \mathrm{g/cm^3}$

* N. R. Shaffer and C. E. Starrett, *Phys. Rev. E* 101, 052304 (2020).
** B. L. Witte et al., *Phys. Plasmas* 25, 056901 (2018).
† A. McKelvey et al., *Sci. Rep.* 7, 7015 (2017).

Stopping power calculations using TD-DFT are a window into dynamic screening physics relevant to conduction electrons

- **Launch a fast test electron into a dense plasma**
- **Energy loss (stopping power) of a test electron is sensitive to the dynamic response of the plasma electrons**
- **Able to capture difficult order-unity dynamic screening corrections to standard Fokker-Planck e-e collision rates**
- **See more in Katarina Nichols's talk this afternoon!**

Stopping Range in Hot Dense CH



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Electron-electron scattering plays essential role in nondegenerate plasma transport

- Lorentz model: e-e collisions maintain local equilibrium (Maxwell-Boltzmann distribution) but do not affect conduction electrons (valid as Z → infinity)
  - N.B. Lee-More is the quantum analogue
- Misses two interconnected effects:
  - Direct e-e scattering influence: compared to e-i collisions, e-e collisions are very effective at changing an electron's energy (important for thermal conduction)
  - Reshaping: conduction electrons are weakly collisional (recall mfp ~ v^4), therefore their distribution is sensitive to the inclusion/neglect of additional collision channels
- Classic result (Spitzer & Harm): neglecting e-e collisions in hydrogen is a 2x error in electrical conductivity and 4x error in thermal conductivity
- In the extreme degeneracy limit, e-e collisions must become negligible. But how quickly is this limit reached in practice? What is the role of e-e scattering at $T \sim E_F$?

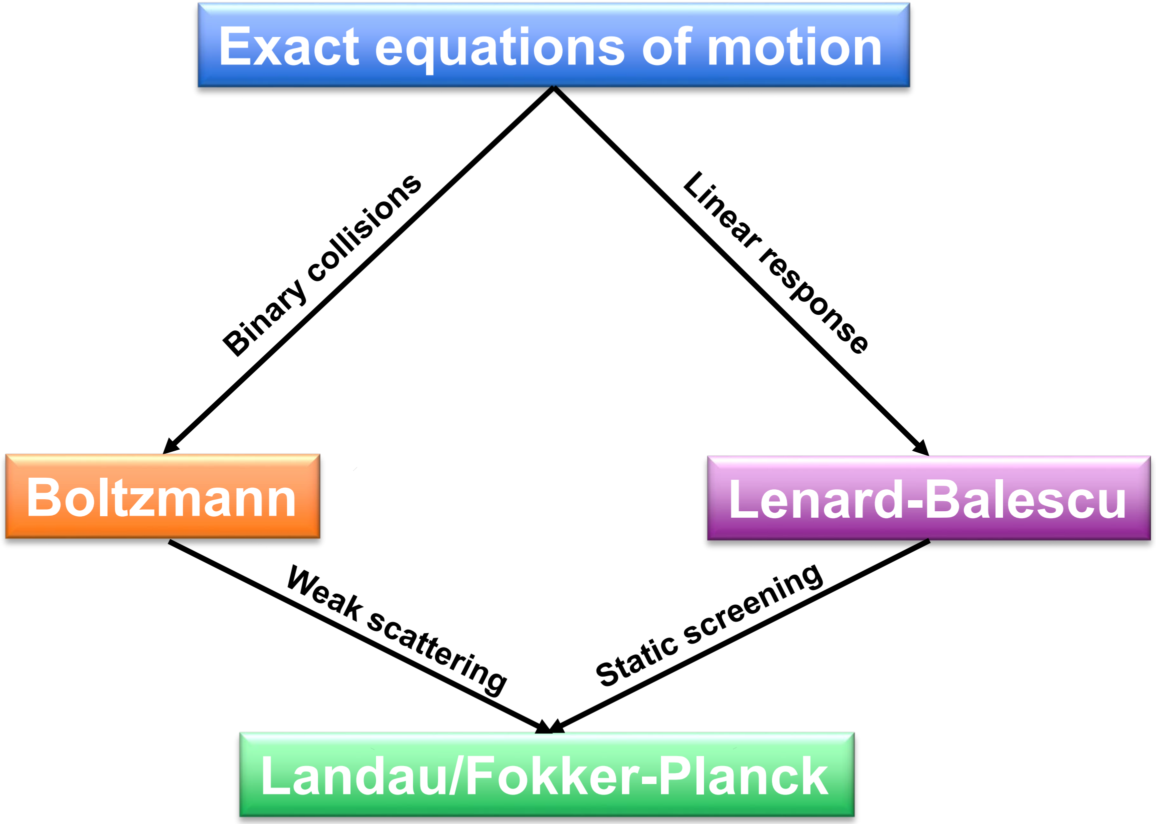
The failure of DFT+KG highlights the need for developing more sophisticated "first principles" calculations for transport properties

- DFT is a theory of fictitious non-interacting electrons – no V_{ee} means no e-e scattering!
  - Hohenberg-Kohn only promises that DFT will deliver an accurate density (or functionals thereof)
  - But Kubo says transport comes from current fluctuations (J(t), Q(t)) which are <u>not</u> density functionals
- What about TD-DFT?
  - Runge-Gross says we can obtain the true J(t) (not sure about Q(t))
  - Requires an accurate *current-density* XC functional, including memory[†]
- In order to capture e-e scattering, our "first-principles" calculations need more principles!
  - Bring V_{ee} back into the picture with many-body perturbation theory?
  - Speculation: focusing on low-frequency phenomena (conduction) might inspire computationally tractable approximations

[redacted]

* J. Dufty et al., *Contrib. Plasma. Phys.* 58, 150 (2017).
** M. French et al., *Phys. Rev. E* 105, 065204 (2022).
† N. Maitra, I. Souza, and K. Burke, *Phys. Rev. B* 68, 045109 (2003).

In the absence of a high-fidelity simulation method, our best available tool is quantum kinetic theory



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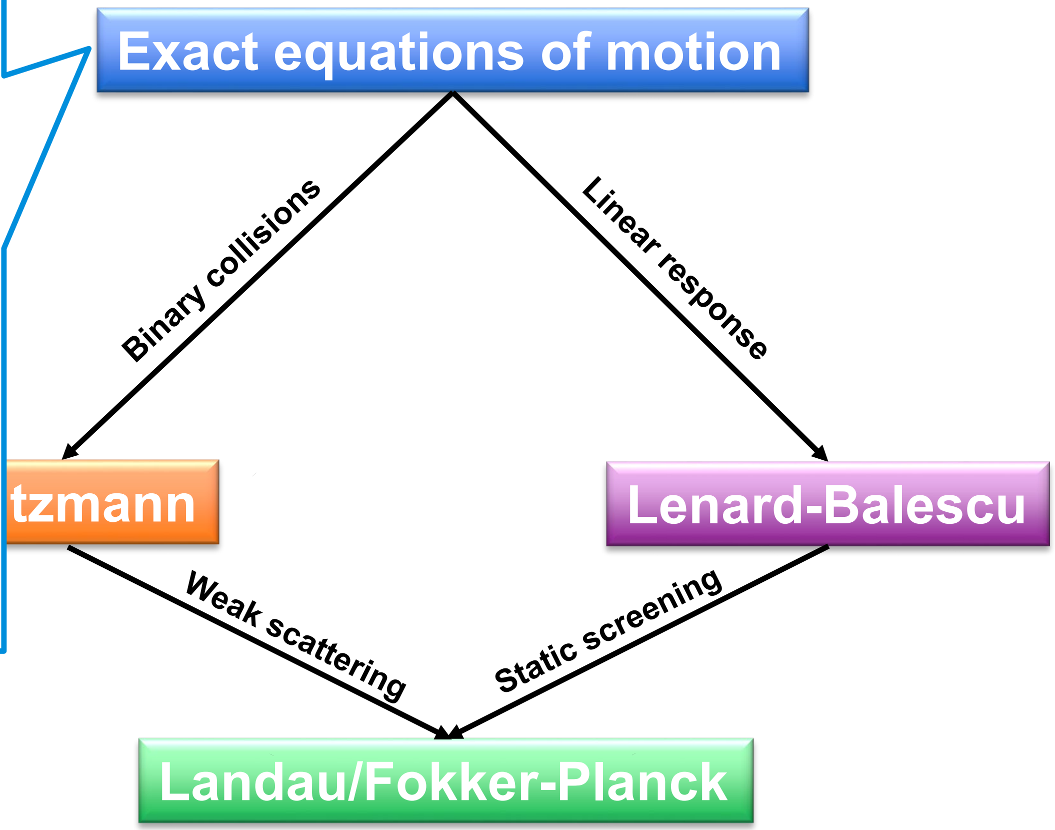
E.g., Kadanoff-Baym

Key quantity: self-energy operator

Includes exchange, correlation, excitations, everything (in principle)!

But very complicated to solve.



* L. P. Kadanoff & G. Baym, *Quantum Statistical Mechanics* (1962).
** A. Stan, N. E. Dahlen, and R. van Leeuwen, *J. Chem. Phys.* 130, 224101 (2009).

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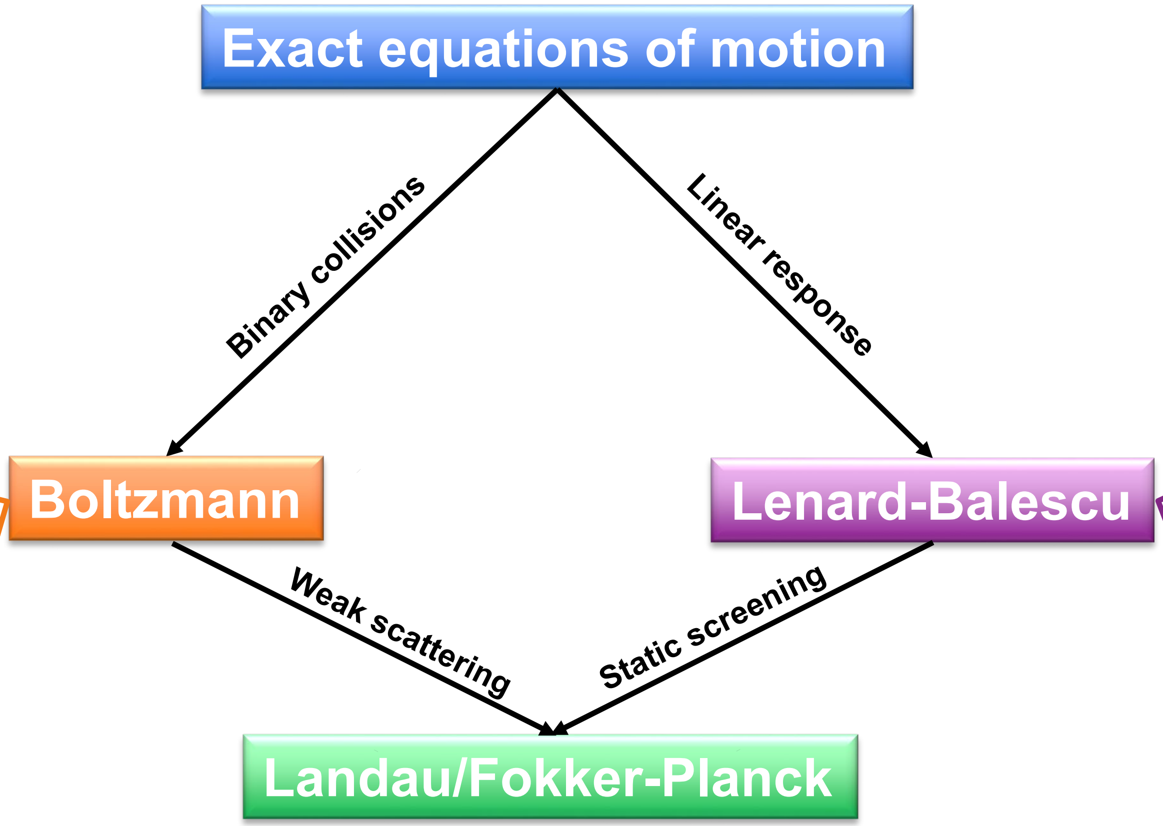
UR LLE

Key quantity: collision cross-section

Solutions known for extreme (non-)degeneracy, but not intermediate



Key quantity: dielectric function

Approximate non-degenerate solutions known, but not for arbitrary degeneracy

"Solution" == "Champan-Enskog solution"

* E. A. Uehling and G. E. Uhlenbeck, *Phys. Rev.* 43, 552 (1933).
** H. Reinholz et al., *Phys. Rev. E* 91, 043105 (2015).
† H. D. Whitley et al., *Contrib. Plasma Phys.* 55, 192 (2015).

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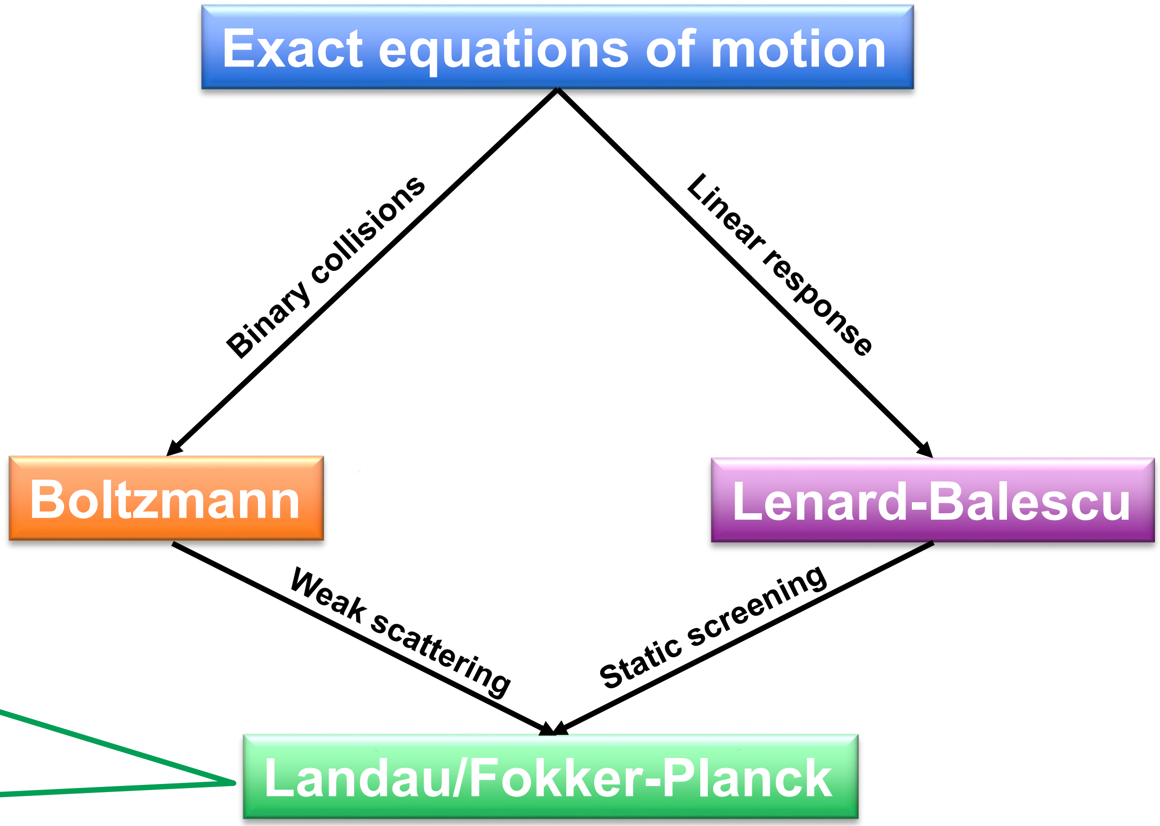

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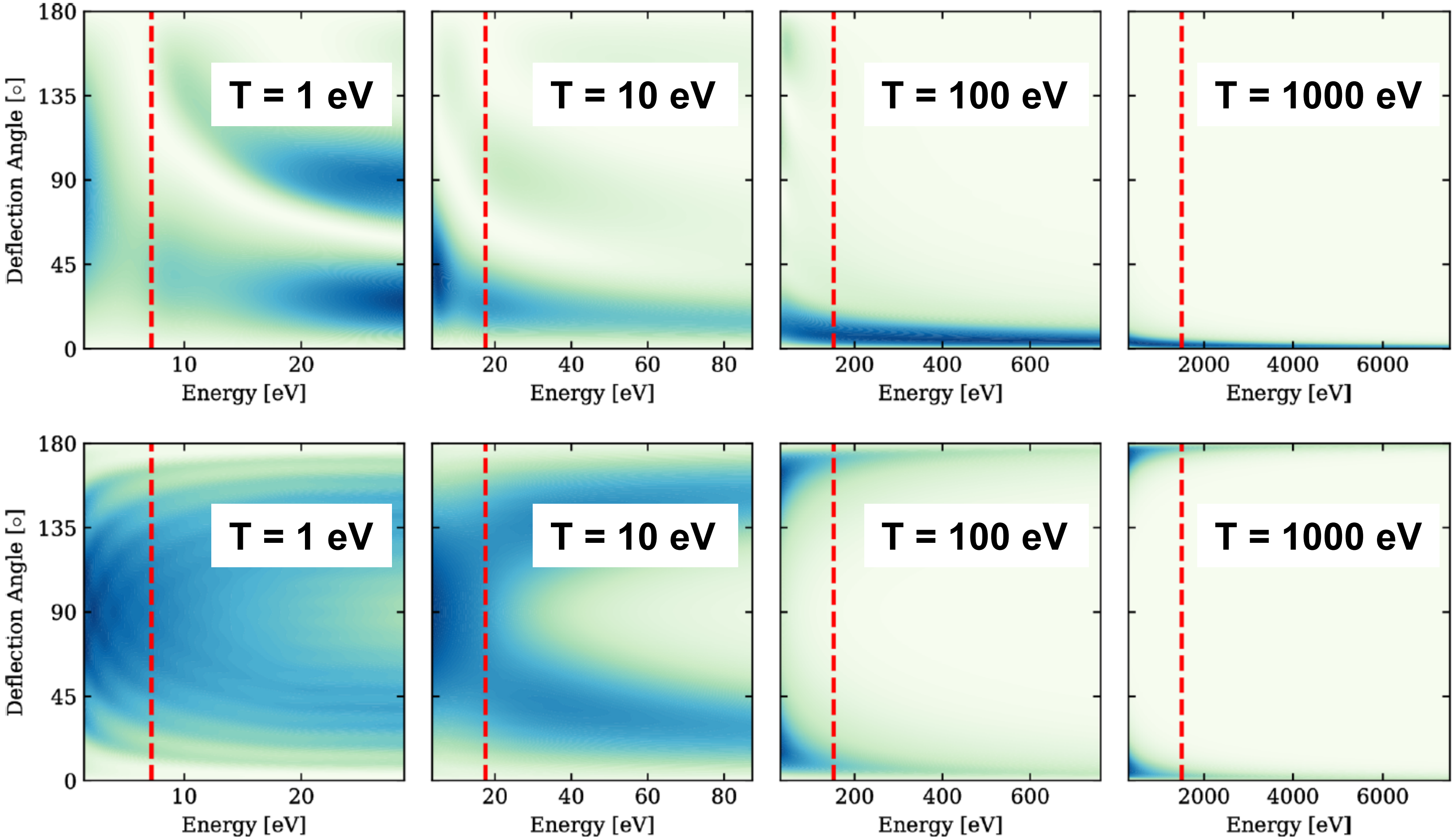
Analysis of scattering angle distributions give insight into the breakdown of the small-angle approximation at low temperatures

e-i

e-e



Solid-density Al

$$D_{ij}(E,\theta) = 2\pi \sin\theta \frac{d\sigma_{ij}}{d\Omega}$$

-- E_{rms}

* N. R. Shaffer and C. E. Starrett, *Phys. Rev. E* 101, 053204 (2020).