Non-equilibrium approaches to averaged properties

Primary Relevance: Statistical Mechanics of Plasmas

Secondary Relevance: Atomic Physics
Transport and Turbulence

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Today I focus on one aspect of one of these five questions

- **How does the exotic behavior of collections of electrons, ions, and photons arise?**
  - **Specific focus here: averaged properties in nonequilibrium**
- **What can creating extraterrestrial plasma conditions in the laboratory reveal?**
- **What can the control and exploitation of transient, intense flows of energy and particles, unconstrained by conventional materials, deliver to science, industry, and medicine?**
- **How can ionized matter be controlled to achieve practical inertial fusion energy?**
- **How does self-organization arise within plasmas?**

There are certain to be omissions and errors here

- **Credit for good stuff**
  - **Dick More**
  - **Justin Wark**
  - **Mike Desjarlais**

- **Credit for wrong stuff: RPD**
  - **Corrections, information, and insight will be welcome**

Tractable theories and simulations are challenged by non-equilibrium effects

$$\frac{\partial}{\partial t}\left\{\begin{array}{c}\rho\\ \rho\mathbf{u}\\ \mathcal{E}+\frac{1}{2}\rho\mathbf{u}\cdot\mathbf{u}\\ \mathcal{E}_e\end{array}\right\}+\nabla\cdot\left\{\begin{array}{c}\rho\mathbf{u}\\ \rho\mathbf{u}\mathbf{u}+p\mathbf{I}\\ \mathbf{u}\left(\frac{1}{2}\rho\mathbf{u}\cdot\mathbf{u}+\mathcal{E}+p\right)\\ \mathbf{u}\mathcal{E}_e\end{array}\right\}=\mathbf{S}$$

laser energy deposition

radiation/electron momentum exchange

electron heat conduction

$$\mathbf{S}=\left\{\begin{array}{c}0\\ -\mathbf{S}_{rm}\\ \nabla\cdot C_e\nabla T_e-S_{re}+S_L\\ -p_e\nabla\cdot\mathbf{u}+\nabla\cdot C_e\nabla T_e+\frac{\rho k_B(T_i-T_e)}{M_pA\tau_{ei}}-(S_{re}-\mathbf{S}_{rm}\cdot\mathbf{u})+S_L\end{array}\right\}$$

Compression work

collisional exchange

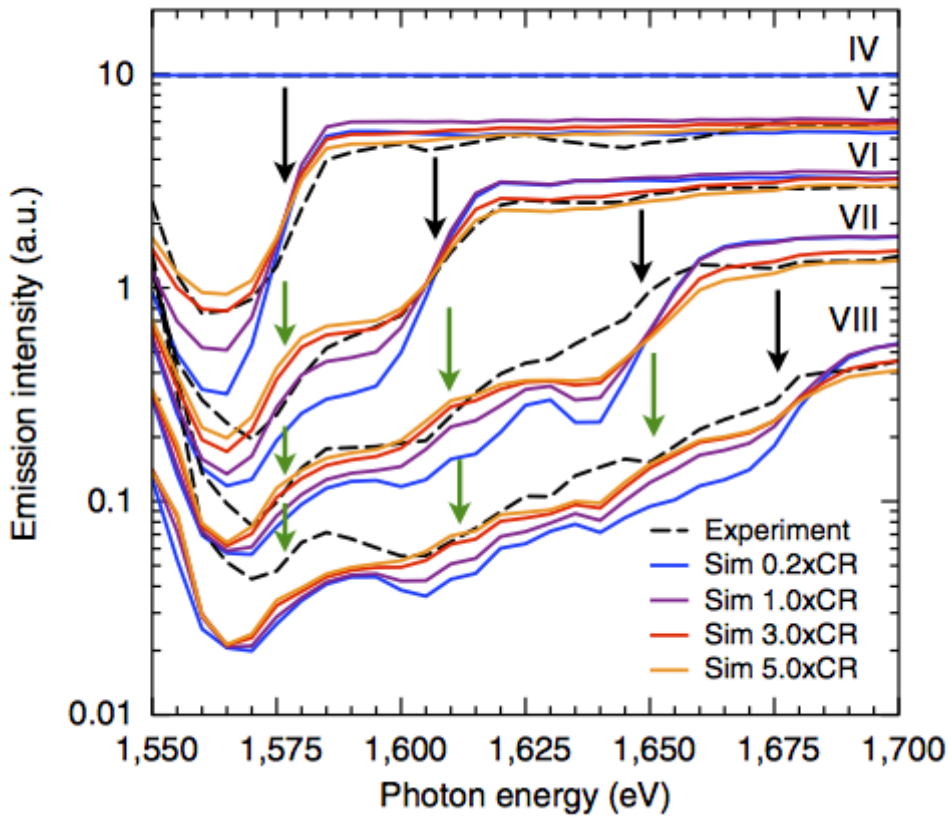
radiation/electron energy exchange

Any such calculation needs a bunch of averaged properties

- Internal energy
- Internal energy in the electrons
- Electron-ion energy exchange rate
- Coefficient(s) for heat conduction
- Coefficients for radiative energy transfer
  - Opacities and/or other quantities
- Ionization and excitation

All of these may differ from their values at equilibrium

Ionization at solid density is faster than predicted by state of the art simulations



K shell emission at solid density involving collisional ionization

Rates simulated by SCFLY model of non-equlibrium state are 5x too small

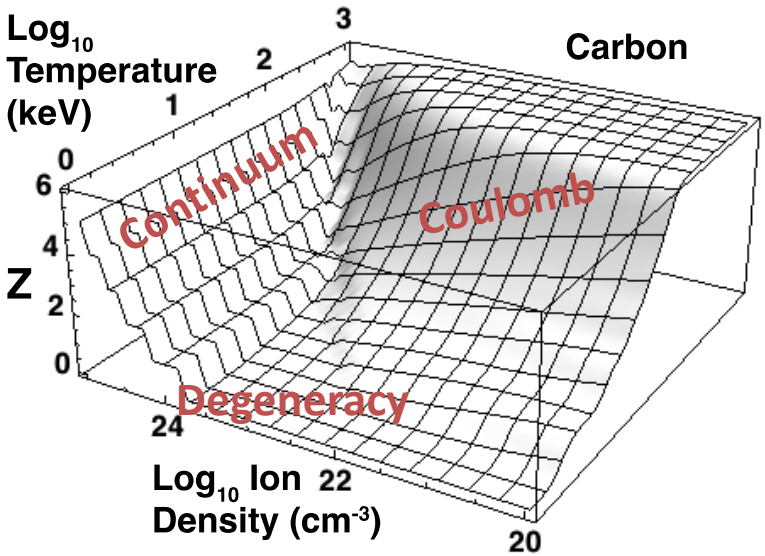
Vinko et al. Nat. Comm. 2015

One of the few experiments about any of this!

Many factors contribute to the properties of dense, non-hydrogenic plasmas p.1

- **Ionization and excitation**
  - The corresponding internal energies can equal the thermal energies
  - Steady nonequilibrium states are common
- **Electron behavior as fermions**
  - Can dominate the plasma pressure but only "free" electrons contribute
  - Relativistic regimes
- **Coulomb interaction energies**
  - Large in "cool" plasmas
  - Affected by quantum behavior in dense, cool plasmas
- **Continuum lowering**
  - Impact on thermal energy density and rate coefficients can be large

Statistical equilibrium plasma model



From Drake, 2nd edition (20xx)

Many factors contribute to the properties of dense, non-hydrogenic plasmas p. 2

- **Photoabsorption rates (opacities)**
  - Strongly affected by ionization
  - Strongly affected by whatever radiation is present
- **Phase changes**
  - Structured solid vs partially ionized molecular "soup" vs ionized "gas"
- **Multiscale motion**
  - Any non-thermal yet non-directed motion (such as turbulence) on unresolved scales takes energy

Kinetic energy amplification when a shock wave interacts with a structured velocity field

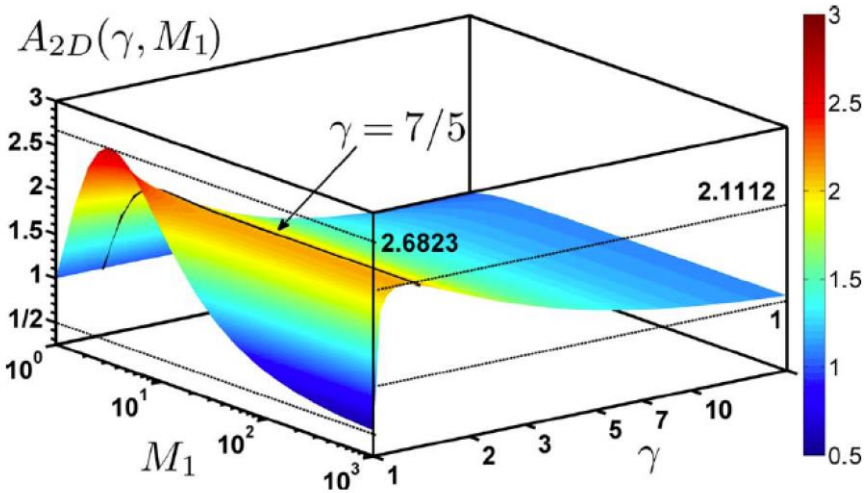


FIG. 30. (Color online) Kinetic-energy amplification factor for a shock interacting with a random 2D vorticity field, as a function of γ and M_1 [Eq. (184)].

Wouchuk et al. PRE 2009

These factors may differ from their equilibrium values, if such even exist

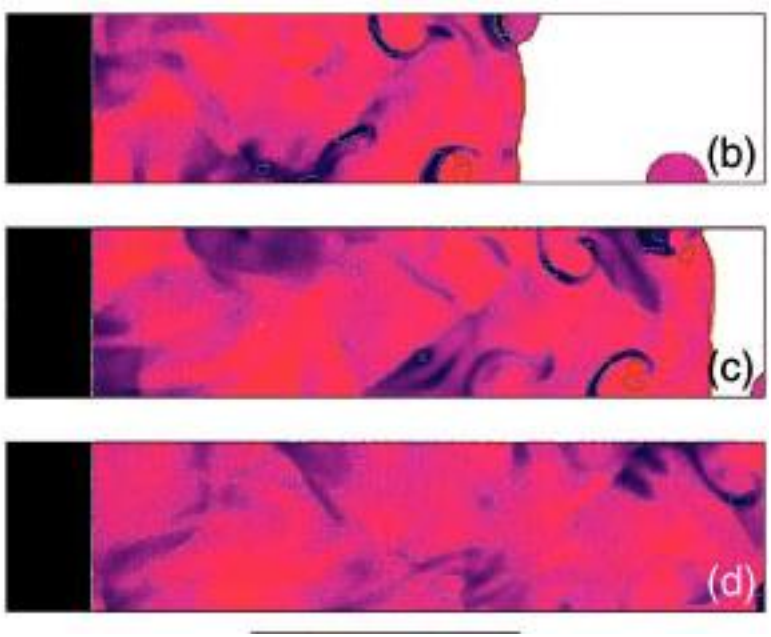
- **Non-equilibrium steady states**
  - **Unequal ion and electron "temperatures"**
  - **Radiation field out of equilibrium**
  - **Ionization state distribution**
  - **Excited state distribution**

- **Non-equilibrium dynamic states**
  - **Multiscale motion**
  - **Rapidly heating plasmas**
  - **Expanding, cooling plasmas**
  - **Plasmas subject to radiation pulses**

Sometimes there is no one equilibrium state

- **Plastics or other complex molecular materials**

- **Foams**
  - **One example of a system with multiscale motions**



Density field in 2D foam model

Led to under-compression, counter-intuitively

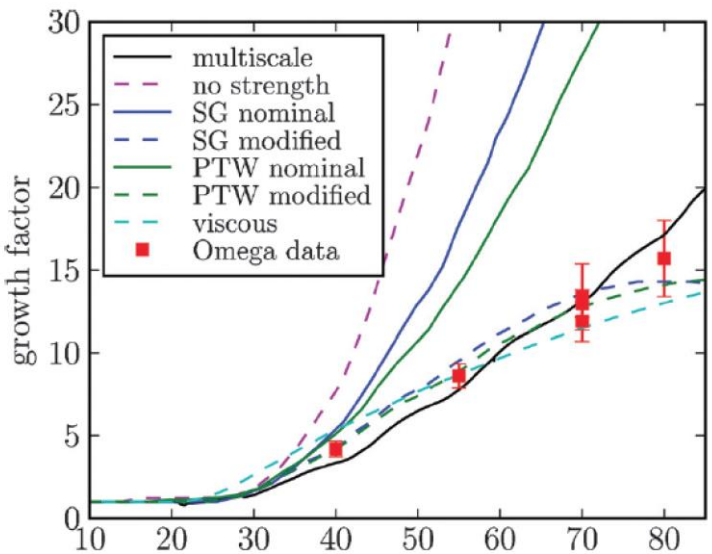
No experiments yet!

Hazak et. al, POP 1998

Approaches to non-equilibrium models

- **Full physics simulations are rarely if ever practical**
  - **Hence the need to treat averaged properties in some way**
  - **Even away from equilibrium**
- **Clever physical models have potential but are little explored**
  - **The big win would be to find new laws from nonequilibrium stat mech**
- **Multiscale methods are promising but very undeveloped**

Growth



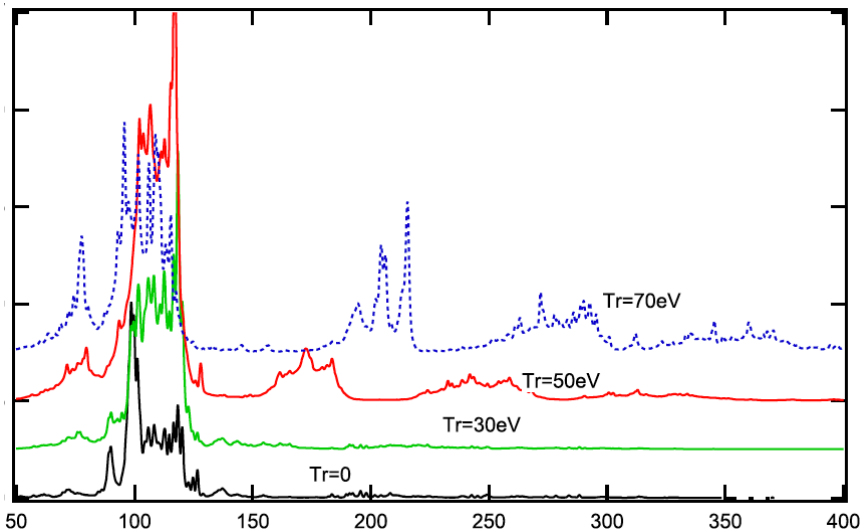
Time (ns)

Multiscale model to address material strength in WDM regime

Barton et al. JAP 2011

There has been work on opacities for steady states away from equilibrium

- Such "Non-LTE" models have been developed for ICF codes.
  - This requires some solution for the ionization state distribution
  - This in turn is affected by the radiation present



Xe emission spectrum from a 100 eV plasma with a blackbody radiation field of various temperatures

Klapisch & Busquet, HEDP 2011

- Some theoretical work involving nonequilibrium stat mech
  - R.M. More and others
- No applications to other thermodynamic parameters
- No experiments

There is scope for a wide range of theoretical and experimental research going forward

- **Relatively complete yet tractable computational models**
  - **Multiscale models**
- **Practical integrated models**
- **Advances in nonequilibrium stat mech and its applications**
- **Experiments to measure the various coefficients under non-equilibrium conditions**
  - **Everywhere from EBIT to X-ray lasers to megajoule lasers**