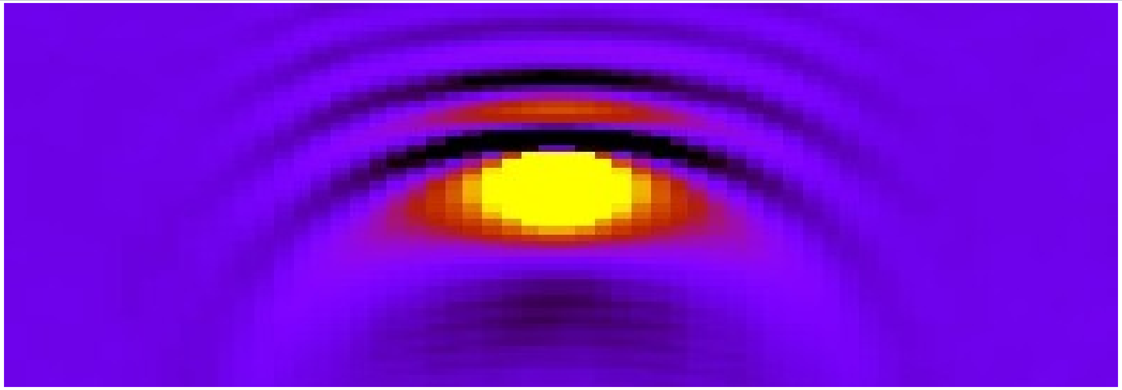
A Many-Body Extension to Madelung Quantum Hydrodynamics



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Collaborators & Acknowledgments

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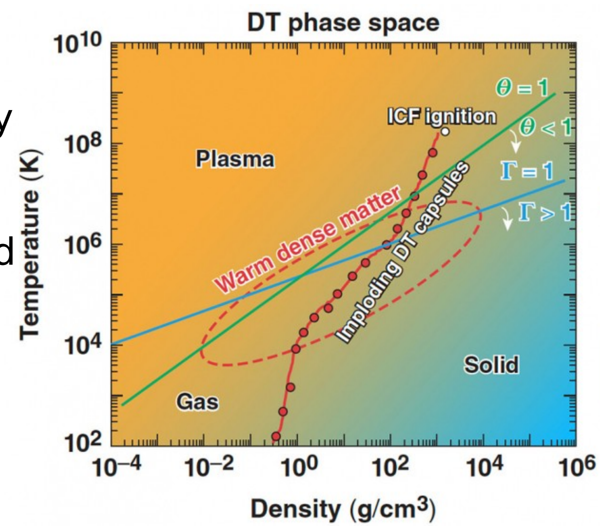
Summary

- Understanding early stages of ICF requires the modeling of charged particle stopping in Warm Dense Matter.
- Quantum Hydrodynamics offers a computationally-efficient treatment of dynamical and quantum-mechanical electrons.
- Here, a QHD model is derived from first-principles, which reproduces Thomas-Fermi degeneracy pressure, a gradient-dependent Bohm pressure, Dirac Exchange potential
- Linearized QHD gives rise to a dimensionless parameter describing the electrons' diffractive character. For projectile stopping, these effects are enhanced and the applicable diffractive region in parameter space is broadened.

Charged Particle Stopping in Warm Dense Matter is important to Inertial Confinement Fusion

- Warm Dense Matter (WDM) occurs in laser and ion-beam plasma experiments, namely early stages of ICF implosion.
- Electrons are moderately Coulomb-Coupled and partially Quantum-Degenerate.
- Can be modeled with: Ab-Initio Molecular Dynamics (MD) with Density Functional Theory (DFT), Quantum Monte Carlo, etc.



1. The Coulomb coupling parameter:

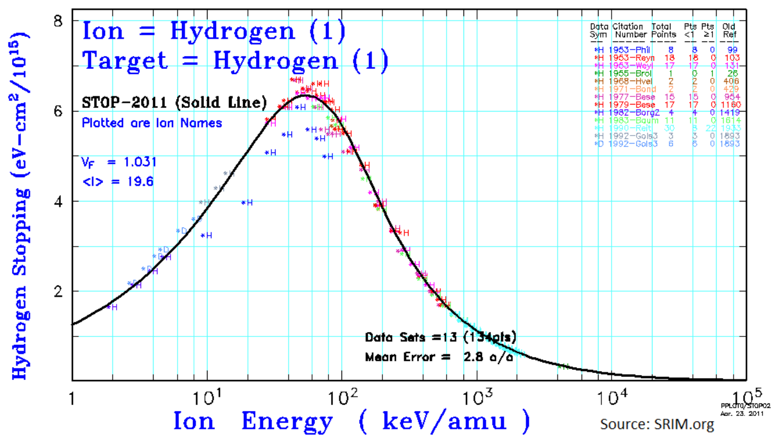
$$\Gamma = \frac{q^2}{r_s k_B T},\ r_s = (3/4\pi n)^{1/3}$$

2. The electron-degeneracy parameter:

$$\theta = \frac{T}{T_F}$$

Warm dense matter (WDM): $\Gamma \geq 1;\ \theta \leq 1$

Source: LLE



- Charged Particle (CP) Stopping of fast alphas is source of bootstrap heating in ICF.
- Stopping of intermediate projectiles near the e- thermal velocity is affected by quantum bound effects.
- **Modeling CP stopping in WDM must include dynamically-screening quantum-mechanical electrons.**

Slow:
Dielectric Fluid

$$-\left.\frac{dE}{dx}\right|_{V \ll v_e} \propto V.$$

Intermediate:
Bound States

Fast:
Binary Scattering

$$-\frac{dE}{dx} = \left(\frac{\omega_p Z e}{V}\right)^2 \ln \Lambda,$$

A Quantum Hydrodynamic approach is well suited for CP stopping in WDM

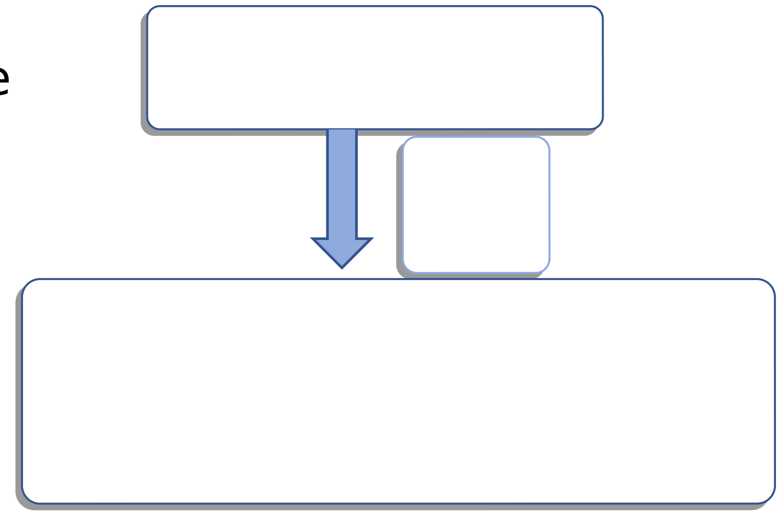
- A quantum electron fluid model can simulate dynamical screening in WDM in a computationally-efficient way.

- Madelung (1927) first proposed this, and proved equivalence between single-particle Schrodinger Equation and Euler Equations.

- Bohm (1952) applied Madelung's approach to many-bodies, but interpreted as deterministically evolving quasi-particle trajectories, instead of hydrodynamically.

- We **need rigorously-derived many-body Quantum Hydrodynamic equations**, in particular generalizing the quantum Bohm potential.

- This is done next.



Many-body Schrodinger Dynamics can be recast as Hydrodynamic Equations

- The Time-dependent Schrodinger Equation is expanded with an N-body Madelung ansatz

$$\Psi_{\mathbf{N}}(\{\mathbf{r}_i\},t) \equiv \sqrt{\frac{n_{\mathbf{N}}}{N}}\exp\left(i\,\frac{S_{\mathbf{N}}}{\hbar}\right)$$

- The 3N-dimensional Density & Action are projected to **3-d fluid quantities**

$$\int\Big(\prod_{j\neq k} d\mathbf{r}_j\Big)\,\frac{\partial n_{\mathbf{N}}}{\partial t} \qquad \int\Big(\prod_{j\neq k} d\mathbf{r}_j\Big)\,\frac{\partial}{\partial t}(n_{\mathbf{N}}\nabla_k S_{\mathbf{N}})$$

- The Quantum evolution satisfies **Hydrodynamic Equations**, with classical and quantum pressure tensors, and external and inter-particle potentials with correlations.

$$\begin{aligned}
\frac{\partial n(\mathbf{r})}{\partial t} + \nabla\cdot\mathbf{j}(\mathbf{r}) &= 0,\\
m\,\frac{\partial \mathbf{j}(\mathbf{r})}{\partial t} + m\,\nabla\cdot\left(\frac{\mathbf{j}(\mathbf{r})\,\mathbf{j}(\mathbf{r})}{n(\mathbf{r})}\right) &= -\nabla\cdot\Big(\mathbf{P}(\mathbf{r}) + \mathbf{Q}(\mathbf{r})\Big) - n(\mathbf{r})\,\nabla V(\mathbf{r})\\
&\quad - (N-1)\int d\mathbf{r}'\; n(\mathbf{r},\mathbf{r}')\,\nabla\phi(|\mathbf{r}-\mathbf{r}'|),
\end{aligned}$$

Wave-function (anti-)symmetry and other constraints are enforced

- Wave Function **(Anti-)Symmetry** is imposed for an arbitrary state

$$n(\mathbf{r}) = \frac{\mathcal{N}}{(N-1)!} \sum_p \sum_q (\pm 1)^{p+q} \int \Big(\prod_{j>1} d\mathbf{r}_j\Big)\, e^{\nu_p+\nu_q} \cos(\sigma_p - \sigma_q),$$
$$\mathbf{j}(\mathbf{r}) = \frac{\hbar}{m} \frac{\mathcal{N}}{(N-1)!} \sum_p \sum_q (\pm 1)^{p+q} \int \Big(\prod_{j>1} d\mathbf{r}_j\Big)\, e^{\nu_p+\nu_q} \Big[\sin(\sigma_p - \sigma_q)\, \nabla\nu_p + \cos(\sigma_p - \sigma_q)\, \nabla\sigma_p\Big],$$
$$\mathbf{K}(\mathbf{r}) = \frac{\hbar^2}{2\,m} \frac{\mathcal{N}}{(N-1)!} \sum_p \sum_q (\pm 1)^{p+q} \int \Big(\prod_{j>1} d\mathbf{r}_j\Big)\, e^{\nu_p+\nu_q} \Big[\cos(\sigma_q - \sigma_p)\,(\nabla\nu_q\nabla\nu_p + \nabla\sigma_q\nabla\sigma_p - \nabla\nabla\nu_p - \nabla\nu_p\nabla\nu_p + \nabla\sigma_p\nabla\sigma_p) + \sin(\sigma_q - \sigma_p)\,(\nabla\nu_q\nabla\sigma_p - \nabla\sigma_q\nabla\nu_p - \nabla\nabla\sigma_p - \nabla\nu_p\nabla\sigma_p - \nabla\sigma_p\nabla\nu_p)\Big].$$

- First approximation: **Slater determinant** of arbitrary single-electron orbitals.

$$n(\mathbf{r}) = \sum_{k=1}^{N} |\chi_k(\mathbf{r})|^2,$$
$$\mathbf{j}(\mathbf{r}) = \frac{\hbar}{m} \sum_{k=1}^{N} |\chi_k(\mathbf{r})|^2\, \nabla\theta_k(\mathbf{r}),$$
$$\mathbf{K}(\mathbf{r}) = \frac{\hbar^2}{2\,m} \sum_{k=1}^{N} |\chi_k(\mathbf{r})|^2 \Big(2\,\nabla\theta_k(\mathbf{r})\nabla\theta_k(\mathbf{r}) - \nabla\nabla\mu_k(\mathbf{r})\Big),$$
$$n(\mathbf{r},\mathbf{r}') = \frac{1}{N-1} \sum_{k=1}^{N} \sum_{k'=1,\neq k}^{N} \Big(|\chi_k(\mathbf{r})|^2 |\chi_{k'}(\mathbf{r}')|^2 - \mathfrak{Re}\, \chi_k^\dagger(\mathbf{r})\, \chi_{k'}(\mathbf{r})\, \chi_{k'}^\dagger(\mathbf{r}')\, \chi_k(\mathbf{r}')\Big).$$

- Orbitals are **Plane-waves** of arbitrary density distribution.

$$\chi_i(\mathbf{r}) \equiv \sqrt{\frac{n(\mathbf{r})}{N}}\, \exp\Big(i\,\mathbf{k}_i \cdot \boldsymbol{\xi}(\mathbf{r}) + i\,u(\mathbf{r})\Big)$$

$$\mathbf{j}(\mathbf{r}) = \frac{\hbar}{m} n(\mathbf{r})\, \nabla\Big(\frac{1}{N} \sum_i \mathbf{k}_i \cdot \boldsymbol{\xi}(\mathbf{r}) + u(\mathbf{r}) \Big)$$
$$\mathbf{P}(\mathbf{r}) + \mathbf{Q}(\mathbf{r}) = \frac{\hbar^2}{m} \frac{n}{N} \Big[\sum_i \big(\nabla\, \mathbf{k}_i \cdot \boldsymbol{\xi}\big)\big(\nabla\, \mathbf{k}_i \cdot \boldsymbol{\xi}\big) - \frac{1}{N} \Big(\sum_i \nabla\, \mathbf{k}_i \cdot \boldsymbol{\xi}\Big)\Big(\sum_i \nabla\, \mathbf{k}_i \cdot \boldsymbol{\xi}\Big) \Big] - \frac{\hbar^2}{4\,m} n\, \nabla\nabla \ln n$$
$$n(\mathbf{r},\mathbf{r}') = \frac{n(\mathbf{r})\, n(\mathbf{r}')}{N} \Big(1 - \frac{1}{N(N-1)} \sum_i \sum_{j\neq i} \cos\big[(\mathbf{k}_j - \mathbf{k}_i) \cdot (\boldsymbol{\xi} - \boldsymbol{\xi}') \big] \Big)$$

Recovers a Bohm pressure of the many-body density

In the Fermi limit, QHD becomes Thomas-Fermi-Bohm-Dirac Hydrodynamics

- Finally, the occupancy of the orbitals is assumed Fermi energy degenerate, and taken in the Local Density Approximation.

- The resulting **Thomas-Fermi-Bohm-Dirac QHD equations** are:

- The Pressure tensor consists of "classical" and quantum terms: Thomas-Fermi, and Bohm, which contains a scaling parameter $1/9 < \lambda < 1$.

- The total Potential consists of the external and mean-field Hartree electrostatic interactions, as well as the Dirac exchange potential.

- Next, their linear response is studied.

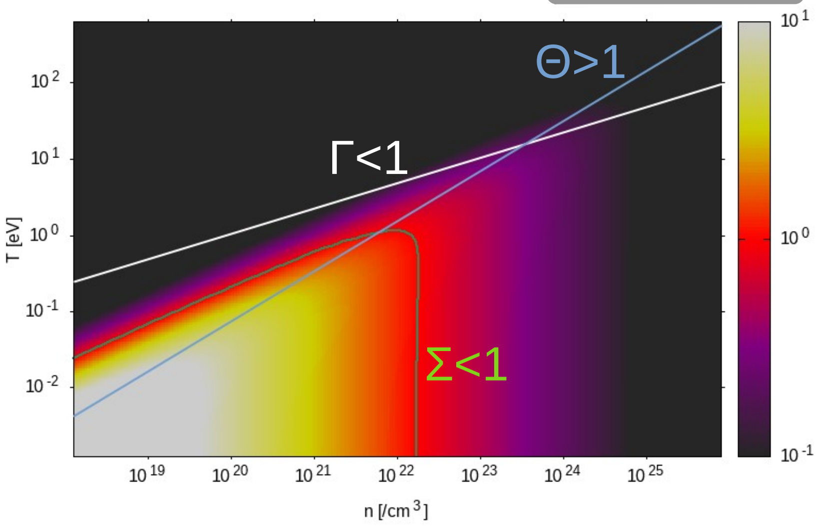
Linearized QHD predicts Screening and Diffractive regimes

- QHD equations can be linearized and solved for Susceptibility/Dielectric. Here, finite-T generalizations (in terms of Fermi Integrals) are used.

- **The Thomas-Fermi length** describes screening, which reduces to Debye in the classical limit.

- **A Kirzhnits length** from the gradient-correction is proportional to particle spacing (degenerate) and de Broglie wavelength (non-degenerate).

Diffractive Parameter:



- A **Dimensionless Diffractive Parameter** describes the character of the plasma response in parameter space.

- $\mathbf{\Sigma_K<1}$: Regular Fermi/Debye exponential screening.

- $\mathbf{\Sigma_K>1}$: Diffractive, stationary Freidel-like spatial oscillations.

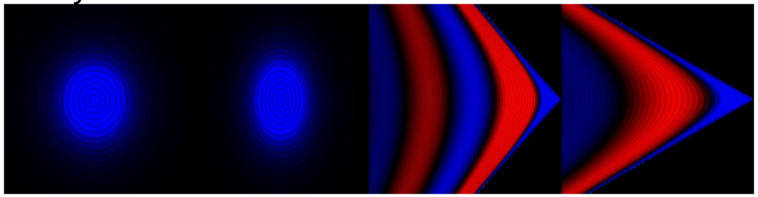
Charged projectile stopping enhances diffractive effects

- Linearized QHD describes Dielectric response to a charged projectile

- The **ratio of projectile to Fermi velocity** characterizes the QHD screening response.

- Thomas-Fermi screening separates into **sub- and super-thermal regimes**

Analytic solutions.



$\beta < 1$ $\beta > 1$

$$\Sigma'_K = \frac{2\lambda_K/\lambda_F}{|\beta^2 - 1|}$$

Simulation with QHD+MD code Nereid.

$\Sigma'_K > 1$

- The **Diffractive Parameter** is modified by the projectile velocity

- Diffractive effects are **enhanced near the Fermi velocity.**

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