Development of a new Quantum Trajectory Molecular Dynamics Framework

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Abstract

The study of matter under extreme pressure conditions is vital for our understanding of the interiors of astrophysical objects[1] – ranging from neutron stars to gas giants like Jupiter – as well as the effort to achieve controlled thermonuclear fusion for energy production via the ICF concept.[2] However, such states can't directly be observed, except at high-power laser facilities where it is transient in nature and only exist for a few billionths of a second and are strenuous to diagnose. Therefore, theoretical and computational work is needed to aid and guide experimental efforts. The regime, commonly referred to as Warm Dense Matter, is challenging to model due to a combination of properties from quantum mechanics – describing everything from molecules to metals – and plasma physics, the physics of stars and the interstellar medium. We are exploring computational techniques not reliant on the Born-Oppenheimer approximation which is commonly employed, where we follow the motion of both the electrons and ions in time. To explicitly follow the election motion is seen to be an important part of describing the dynamical properties of the dense plasma e.g., electrical conductivity or mass diffusion.[3]

Motivation

- Laboratory astrophysics
  → Create conditions found in stars and gas giants
- What is the internal structure of Jupiter?[4]

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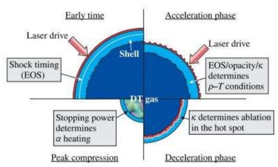

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- **I**nertial **C**onfinement **F**usion
- Fusion by laser compression
- Can the fuel compression be predicted and optimised?[5]

Warm Dense Matter

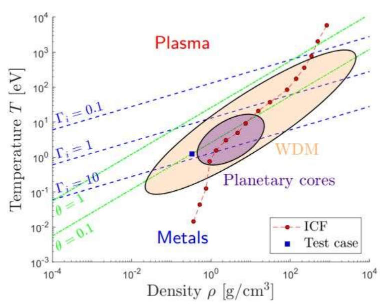
- Strong ion correlations

$$\frac{\text{Potential energy}}{\text{Kinetic energy}} \approx 1$$

$\Rightarrow$ Correlated and collective motion – Liquid-like

- Quantum effects

$$\frac{\text{Temperature}}{\text{Fermi temperature}} \lesssim 1$$



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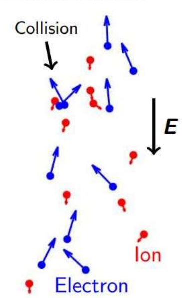
Unknown Physical Properties

Many physical properties are still partially or fully unknown:

- Equations of State – $P = P(T, \rho)$
- Ionic sound speed – Wave propagation
- Mass diffusion – Mass spread
- Electrical resistivity – Resistance to electrical current
- Thermal conductivity – Heat flow

Electrical current



Microscopic modeling

Follow the classical microscopic motion of electrons and ions

$$\frac{\partial \boldsymbol{x}_i}{\partial t} = \boldsymbol{v}_i$$

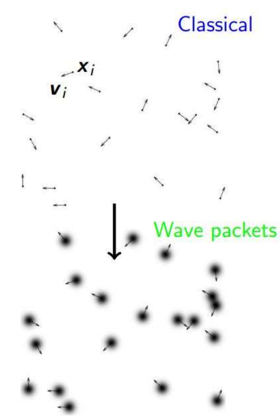
$$\frac{\partial \boldsymbol{v}_i}{\partial t} = \boldsymbol{F}_i$$

based on interactions $\boldsymbol{F}_i$.

Quantum dynamics by the Schrödinger equation,

$$i\hbar\frac{\partial \psi}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial^2 \boldsymbol{x}}\psi + V(\boldsymbol{x})\psi$$

approximate with distributed wave packets.



Extended Wave Packet Model

Extend the functional form of the wave packet by the introduction of elongation

$$\psi \propto \exp\left[-\boldsymbol{\xi}_i^{\mathsf{T}}\left(\frac{\boldsymbol{\Sigma}_i^{-1}}{4} - \frac{im\boldsymbol{\Pi}_i}{\hbar}\right)\boldsymbol{\xi}_i + \frac{im}{\hbar}\boldsymbol{v}_i^{\mathsf{T}}\boldsymbol{\xi}_i\right]$$

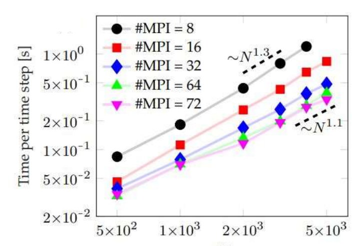
where $\boldsymbol{\xi}_i = \boldsymbol{x} - \boldsymbol{r}_i$ and described by

- $\boldsymbol{r}_i$ – Position
- $\boldsymbol{v}_i$ – Velocity
- $\boldsymbol{\Sigma}_i$ – Width and rotation
- $\boldsymbol{\Pi}_i$ – Speed of width and rotation

Scalable Numerical Implementation

The wave-packet model is natively implemented in LAMMPS[6]

- Parallel program by MPI
- Treatment on many particles N, $N \sim 1000$
- Close to linear scaling w. N
- Custom exchange interactions[7]

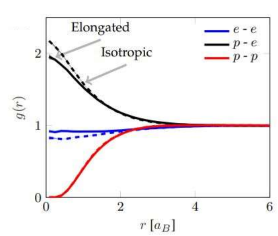


Electronic correlations

Correlated plasma particles:

$$g_{ab}(r) \approx \begin{cases} > 1 & \text{Excess } a\text{-particles} \\ < 1 & \text{Deficit } a\text{-particles} \end{cases}$$

at a distance r from a b particle.



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This work was supported by AWE UK and Oxford Physics Endowment for Graduates (OXPEG)