

Yale

Lawrence Livermore
National Laboratory



Simulating Quantum High Energy Density Plasmas: Approximations According to the Time-Dependent Variational Principle

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with contributions from

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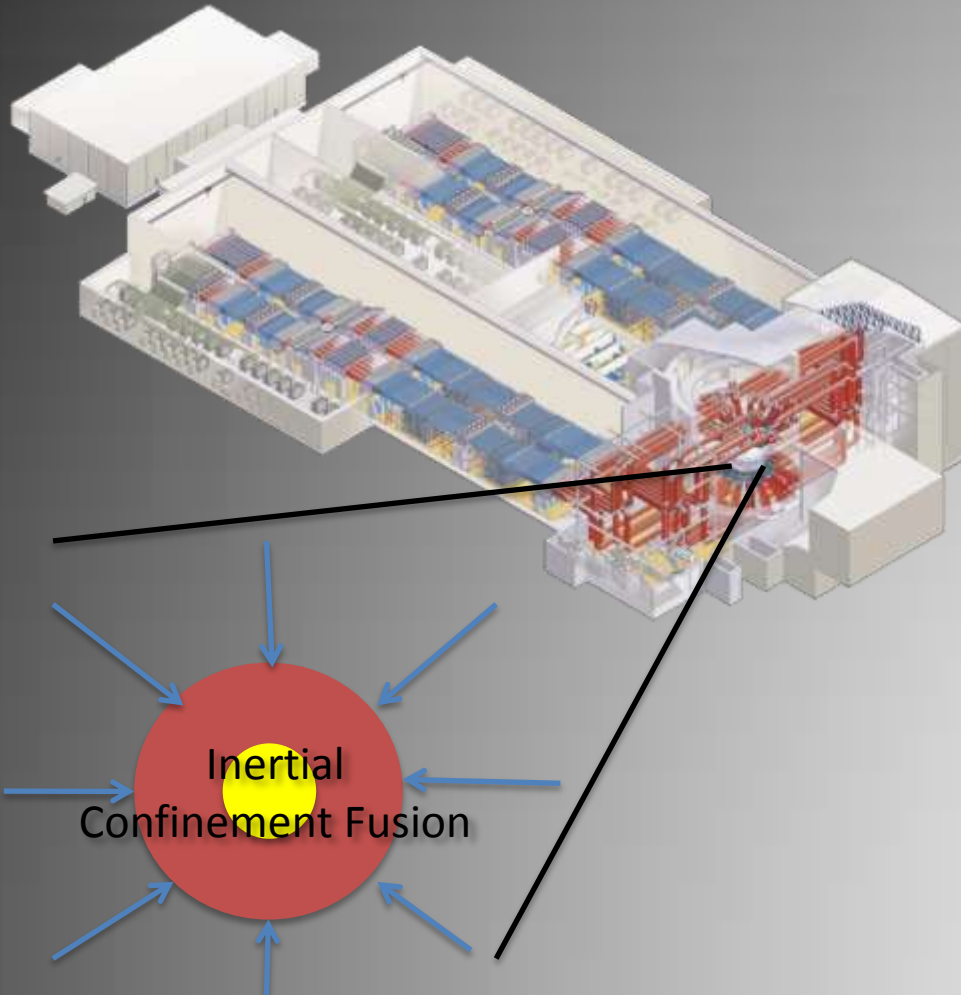
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Heather Whitley (LLNL), Lorin Benedict (LLNL), David F. Richards (LLNL),

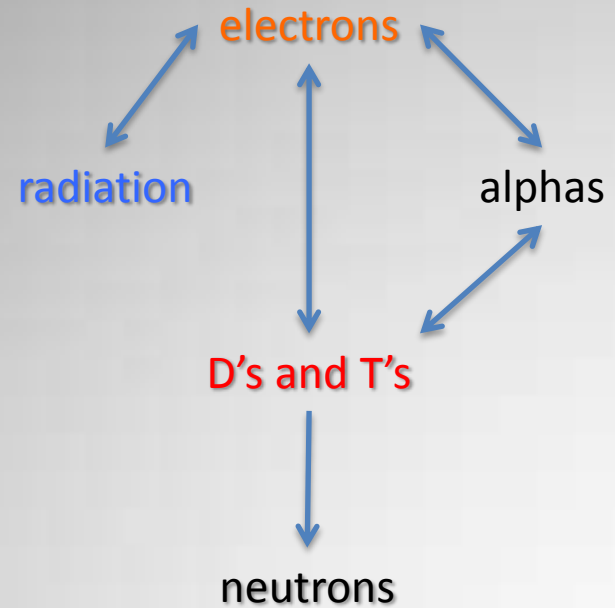
Igor Morozov (RAS), Ilya Valuev (RAS), Victor S. Batista (Yale), Frank R. Graziani (LLNL)

Motivation

National Ignition Facility

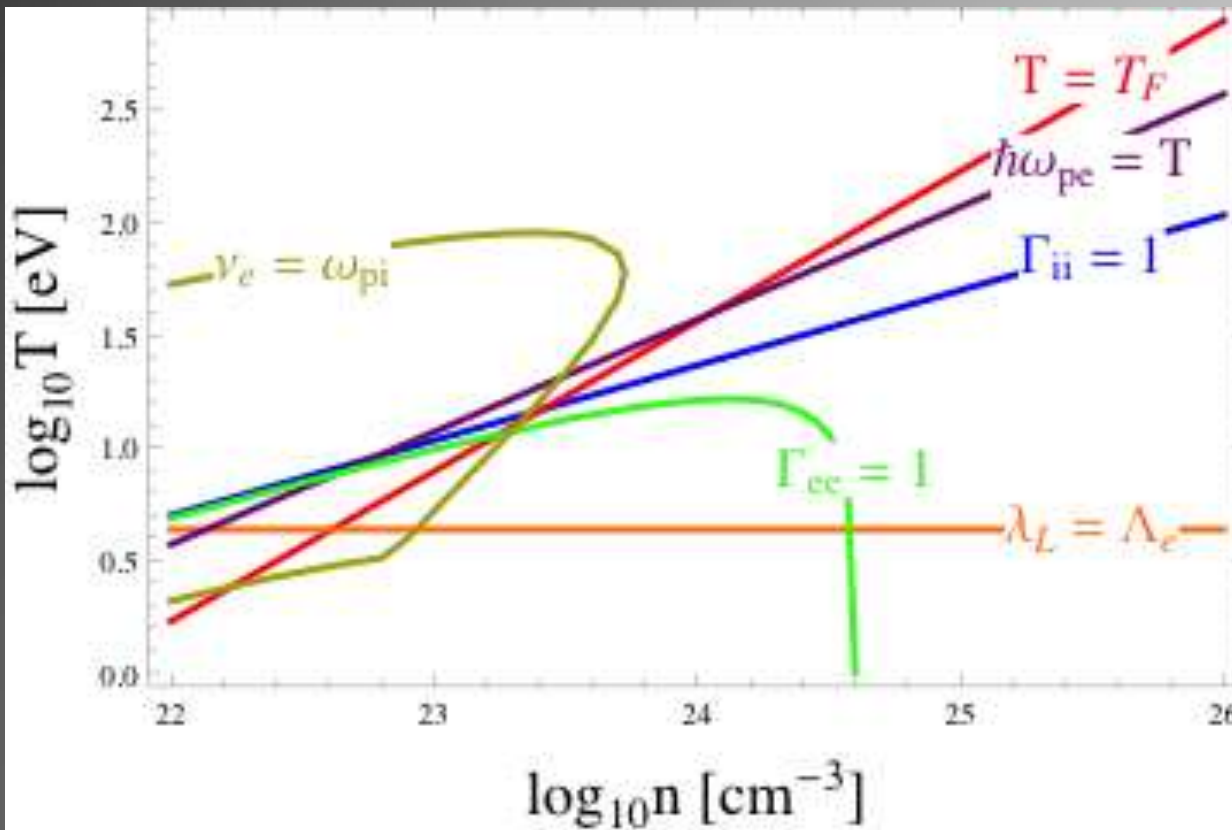


Energy Balance



The high densities ($10^{24-26} \text{ cm}^{-3}$) imply that quantum mechanics is necessary for the electrons.

Quantum Effects

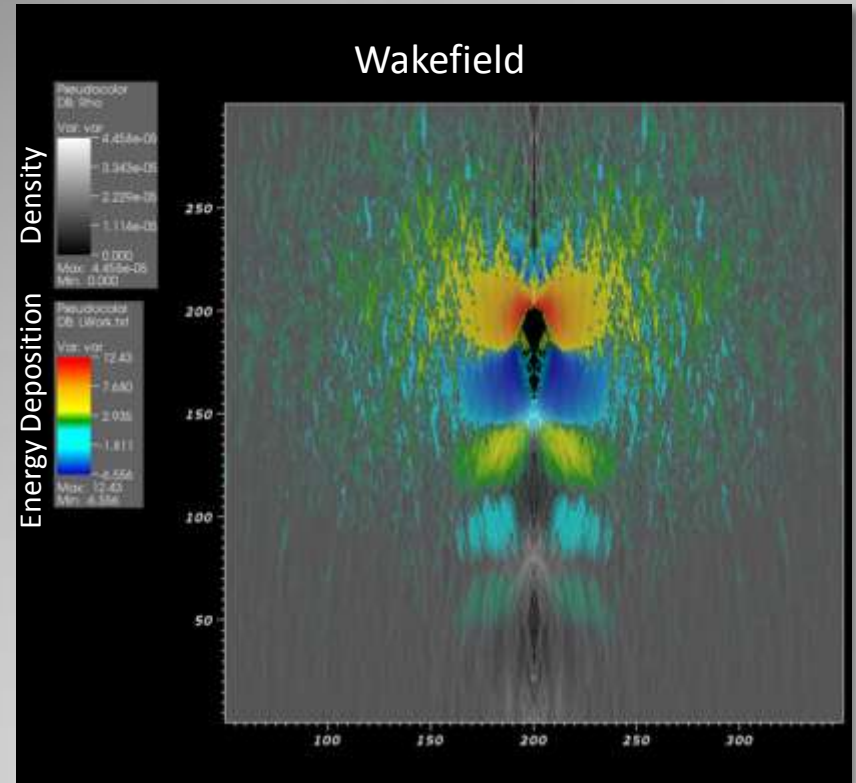
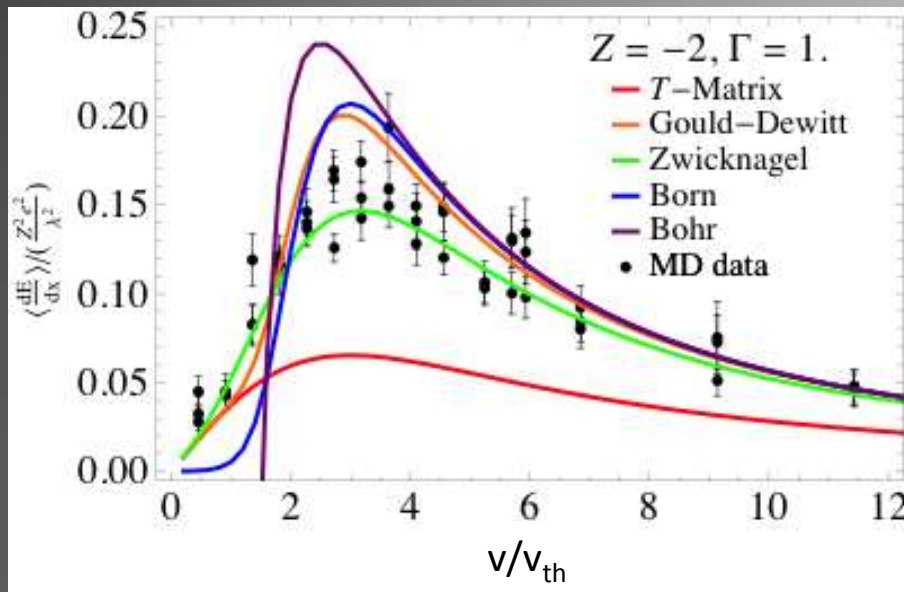


- Ion Coupling
- Electron Coupling
- Degeneracy
- Coulomb Logarithm
- Dynamic Response
- Adiabaticity

Stopping Power

Large discrepancies exist between theoretical models

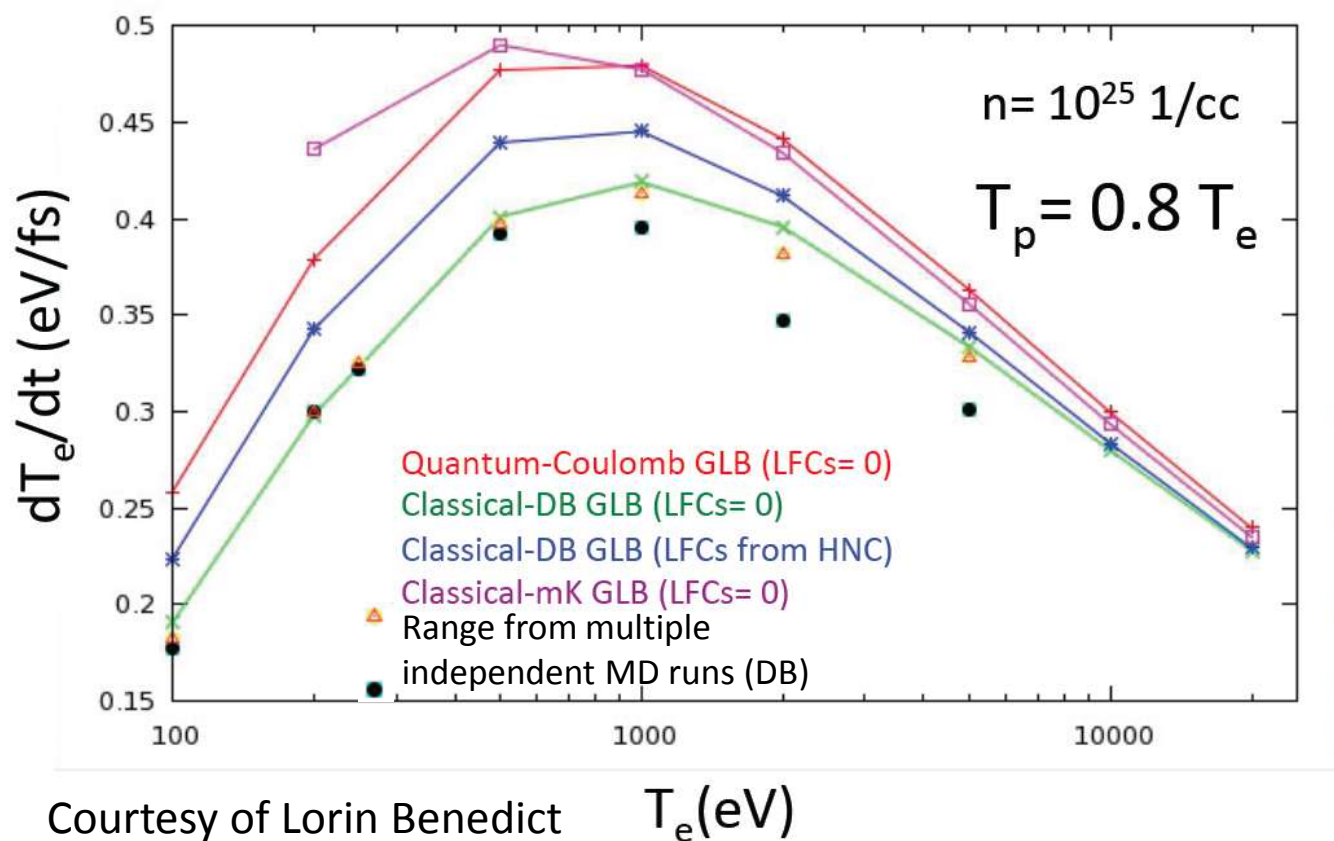
Classical Stopping



We need a computational tool capable of distinguishing between models for quantum stopping

MD Simulations by Mike Surh

Temperature Relaxation



Potentials

DB = Dunn-Broyles
mK = modified Kelbg
(using exact pair density matrix)

Kinetic Models

GLB = Generalized Lennard-Balescu
LFC = Local Field Correction

Methods

MD = Molecular Dynamics
HNC = Hypernetted Chain

HNC provides a static LFC from a potential. MD gives a dynamic LFC implicitly.

How well do quantum statistical potentials calculate temperature relaxation?

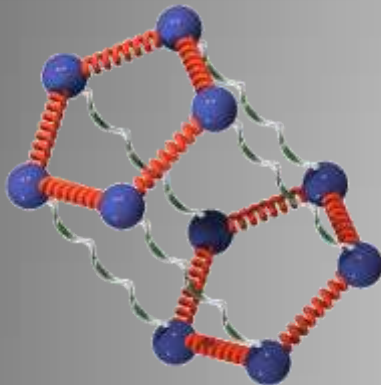
How important are local field corrections?

How important is quantum dynamic response?

Path Integral Monte Carlo

$$\begin{aligned} Z &= \int d\mathcal{R} \langle \mathcal{R} | e^{-\beta \hat{H}} | \mathcal{R} \rangle \\ e^{-\beta \hat{H}} &= (e^{-\beta \hat{H}/P})^P \\ Z &= \int d\mathcal{R} \langle \mathcal{R} | (e^{-\beta \hat{H}/P})^P | \mathcal{R} \rangle \\ &= \int d\mathcal{R} \dots d\mathcal{R}_{P-1} \langle \mathcal{R} | \dots (e^{-\beta \hat{H}/P}) | \mathcal{R}_1 \rangle \langle \mathcal{R}_1 | (e^{-\beta \hat{H}/P}) | \mathcal{R} \rangle \end{aligned}$$

This leads to the “polymer ring isomorphism”:

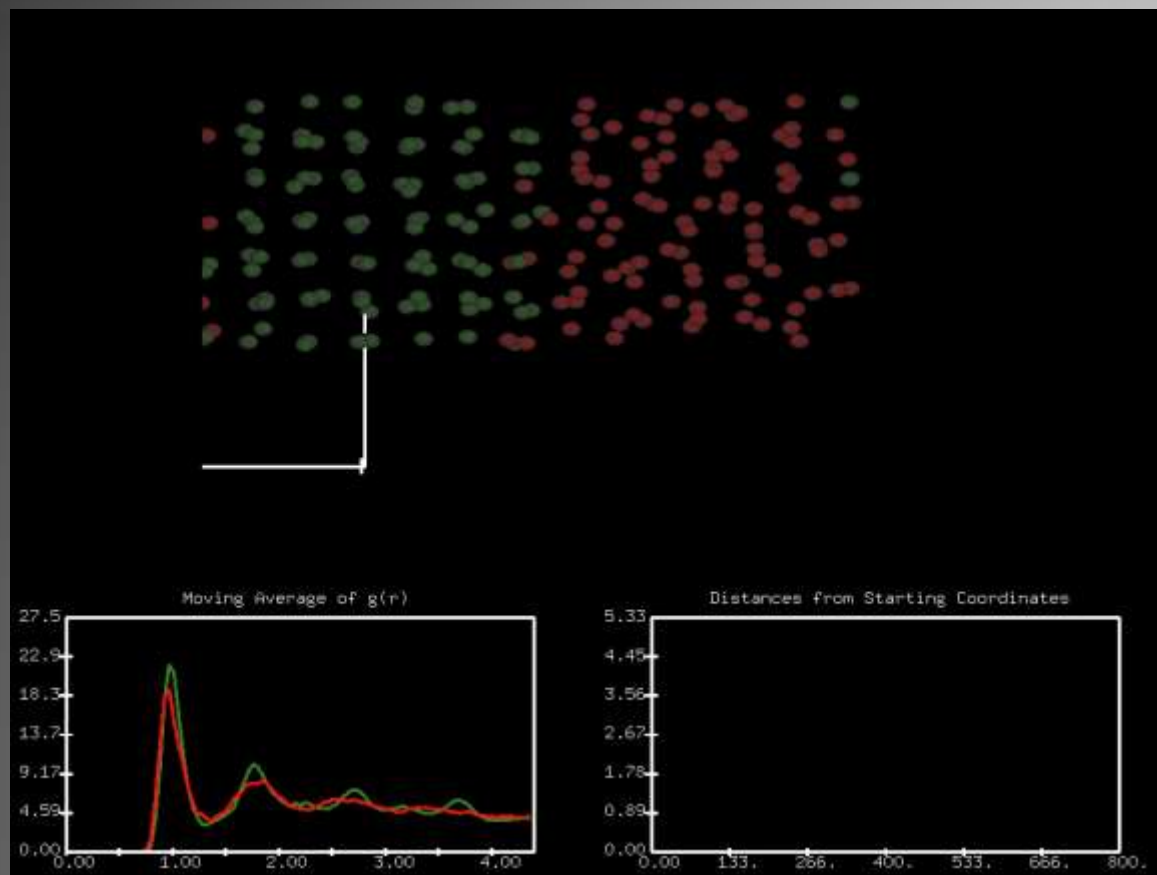


Main difficulty is the Fermion Sign Problem.

Highly Accurate, but computationally demanding and limited to equilibrium

Quantum Molecular Dynamics

Xenon melting, $n = 9.91 \text{ g/cc}$, $T = 6000\text{K}$



Green atoms are initially solid
Red are initially liquid

- Great static electron and dynamic ion properties
- Great dynamic properties near equilibrium within linear response
- Adiabatic approximation

Courtesy of Luke Shulenburger

Quantum Statistical Potentials (QSPs)

MD codes are designed to solve a classical problem. Can we make quantum mechanics look like classical mechanics?

Utilize well-known properties of the quantum partition function.

$$\begin{aligned} Z &= \sum_s e^{-\beta E_s} \\ &= \sum_s \langle s | e^{-\beta \hat{H}} | s \rangle \\ &= \text{Tr} \left[e^{-\beta \hat{H}} \right] \\ &= \int d\mathcal{R} \langle \mathcal{R} | e^{-\beta \hat{H}} | \mathcal{R} \rangle \end{aligned}$$

$$\beta = (k_B T)^{-1}$$

$$\hat{H} = \hat{T} + \hat{U}$$

$$|\mathcal{R}\rangle = |\mathbf{r}_1, \mathbf{r}_2, \dots, \mathbf{r}_N\rangle$$

Classical mechanics looks similar....

$$Z_{CM} = \frac{1}{N!(2\pi\hbar)^{3N}} \int d^{3N}p d^{3N}r \exp \left[-\beta \left(\sum_i \frac{p_i^2}{2m_i} + \sum_{i<j} U(r_{ij}) \right) \right]$$

Defining the QSP Formally

Key observations:

1. Gaussian integrals in classical form are trivially done.
2. Expectation of density operator is positive.

$$\begin{aligned} Z &= \int d\mathcal{R} \langle \mathcal{R} | e^{-\beta \hat{H}} | \mathcal{R} \rangle \\ &= \mathcal{C} \int d^{3N} p d\mathcal{R} e^{-\beta T_{CM}} \langle \mathcal{R} | e^{-\beta \hat{H}} | \mathcal{R} \rangle \\ &= \mathcal{C}' \int d^{3N} p d\mathcal{R} e^{-\beta T_{CM}} \frac{\mathcal{C}}{\mathcal{C}'} \langle \mathcal{R} | e^{-\beta \hat{H}} | \mathcal{R} \rangle \\ &\equiv \mathcal{C}' \int d^{3N} p d\mathcal{R} e^{-\beta(T_{CM} + U(\mathcal{R}))} \\ \mathcal{C}' &= \frac{1}{N!(2\pi\hbar)^{3N}} \end{aligned}$$

Multiplying by one

The many-body potential

$$\frac{\mathcal{C}}{\mathcal{C}'} \langle \mathcal{R} | e^{-\beta \hat{H}} | \mathcal{R} \rangle \equiv e^{-\beta U(\mathcal{R})}$$

Three approximations:

1. Assume antisymmetry is additive: *Pauli potential*
2. Assume that total interaction is sum over pairs: *diffractive potential*
3. Assume system is near equilibrium

Density Dependent Pauli Potentials

- For a finite temperature and density *ideal* Fermi gas, the effective potential can be explicitly written down.
- In a pair approximation, the effective interaction results from the solution of a non-linear integral equation.
- We solved that equation and we fit the result.
- *Important point:* we fit to a density-dependent pair potential.

Pauli potential:

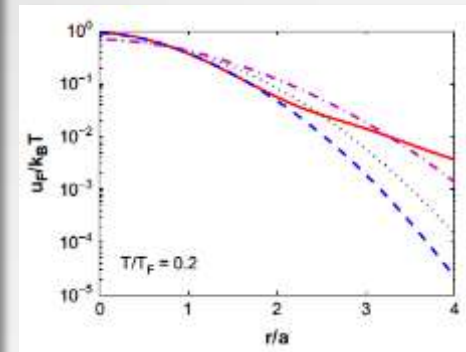
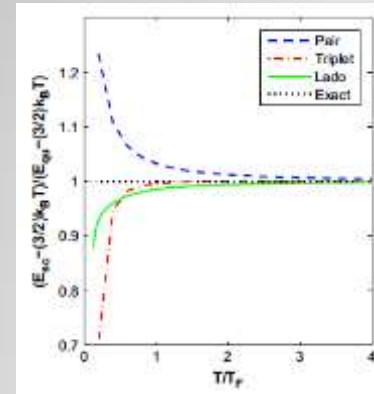
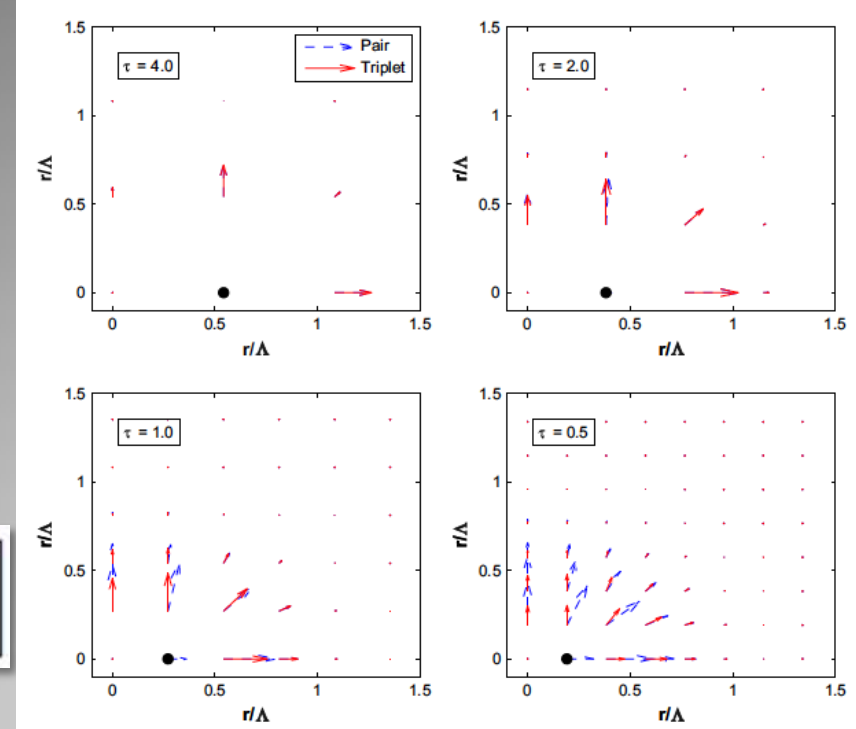
$$u_2(r) = -k_B T \ln \left[1 - \frac{1}{2} A(\tau) \exp(-2\pi B(\tau) r^2 / \Lambda^2) \right]$$

Definitions used:

$$A(\tau) = 1 + \frac{a_1}{1 + a_2 \tau^{a_3}}, \quad B(\tau) = 1 + b_1 \exp(-b_2 \tau^{b_3}) / \tau^{b_4}$$

$$\Lambda = \sqrt{2\pi \hbar^2 / k_B T m}$$

$$\tau = \frac{T}{T_F} \propto \left(\frac{a}{\Lambda} \right)^2$$



Available online at www.sciencedirect.com

ScienceDirect

High Energy Density Physics

High Energy Density Physics 5 (2007) 379–394

www.elsevier.com/locate/hedp

Analysis of semi-classical potentials for molecular dynamics and Monte Carlo simulations of warm dense matter

Christopher S. Jones ^{a,*}, Michael S. Murillo ^b

Great paper for learning QSPs

Public Release number LA-UR-12-21648 Paul E. Grabowski

Pair Diffraction Potentials

Solve the Bloch equation perturbatively:

$$\begin{aligned}\hat{\rho} &= e^{-\beta\hat{H}} \\ \frac{\partial\hat{\rho}}{\partial\beta} &= -\hat{H}\hat{\rho} \\ &= -(\hat{T} + \hat{U})\hat{\rho}\end{aligned}$$

→ Kelbg potential

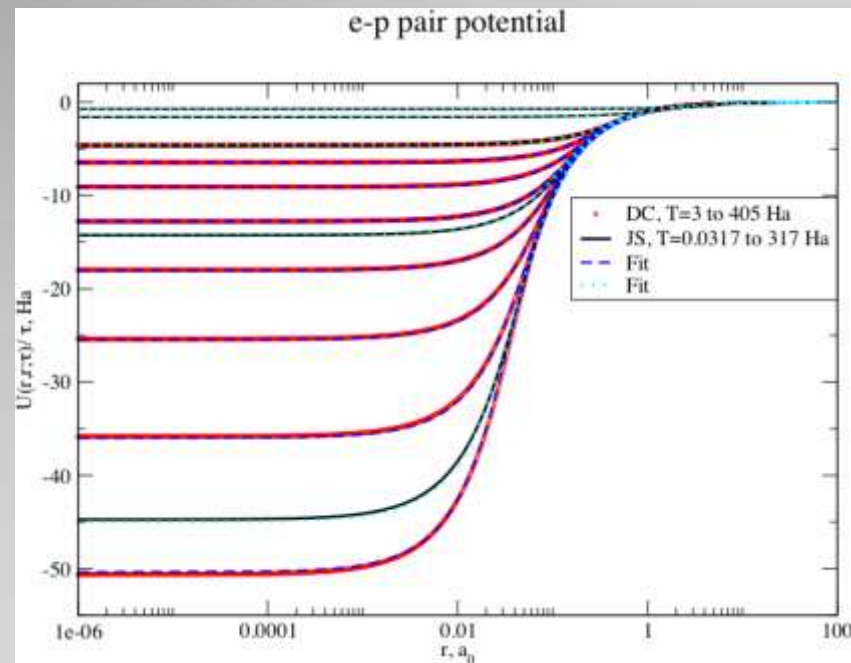
There is no reason not to simply solve this exactly, using solutions of the two-body Schrodinger equation:

$$\rho_2(r, r'; \beta) \equiv \sum_s \psi_s(r) e^{-\beta E_s} \psi_s^*(r')$$

$$V_{eff}(r, \beta) = -\frac{1}{\beta} \ln \left(\frac{\rho_2(r, r; \beta)}{\rho_1(r, r; \beta)} \right)$$

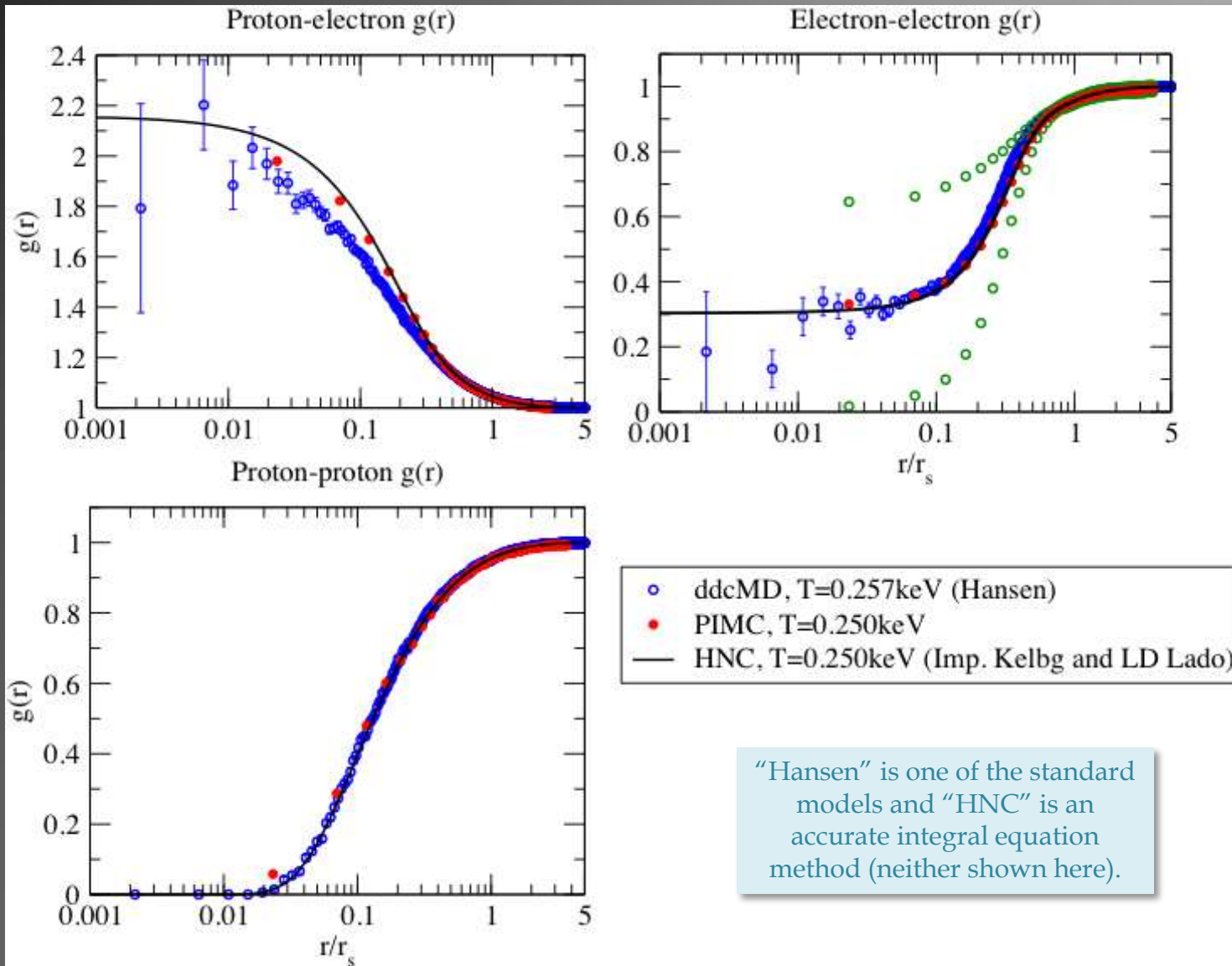
$$V_{eff}(r) = \frac{q_1 q_2}{r} \left[1 - e^{-\left(\frac{r}{\lambda}\right)^2} + \frac{r}{\lambda \gamma} \sqrt{\pi} \left(1 - \operatorname{erf} \left(\gamma \frac{r}{\lambda} \right) \right) \right]$$

We include contributions from the discrete and continuous spectrum (i.e., bound states are included).



Courtesy of Michael S. Murillo and Heather Whitley

Results for Hot Dense Hydrogen



$$\Gamma_{ei} = 0.01$$
$$\theta = \frac{T}{T_F} = 6.05$$

“Hansen” is one of the standard models and “HNC” is an accurate integral equation method (neither shown here).

Successes and Failures of QSPs

Why QSPs work.

$$S(k, \omega) = \mathcal{C} \int_{-\infty}^{\infty} dt \langle n(k, t) n(-k, 0) \rangle e^{i\omega t}$$

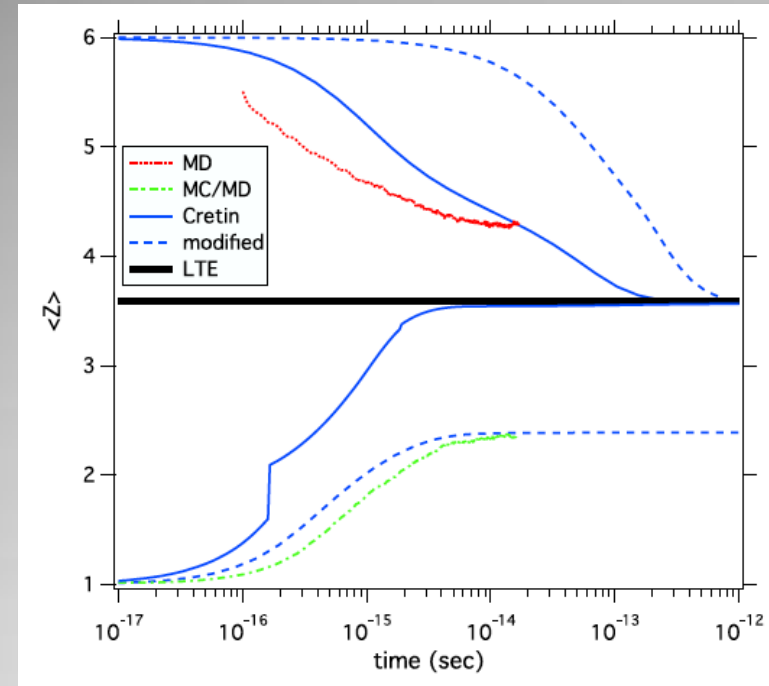
$$S_{ee}(k, \omega) = -\frac{\hbar\omega_{pe}}{\pi n_e \left(1 - \exp\left(-\frac{\hbar\omega}{T_e}\right)\right)} \text{Im} \left[\frac{\chi_0^{\text{HT}}(k, \omega)}{1 - v(k) \chi_0^{\text{HT}}(k, \omega)} \right]$$

$$\text{Im} [\chi_0^{\text{HT}}(k, \omega)] = -\frac{2n_e\beta\omega}{k} \sqrt{\frac{\pi\beta m_e}{2}} \exp\left(-\frac{\beta m_e \omega^2}{2k^2} - \frac{\beta \hbar^2 k^2}{8m_e}\right) \frac{\sinh\left(\frac{\beta \hbar \omega}{2}\right)}{\beta \hbar \omega}$$

This term acts to suppress unphysical density fluctuations (Heisenberg).

Dynamic quantum response differs from classical response

Why QSPs don't work.



Atomic recombination in carbon.

Excellent static properties, but dynamic properties need to be checked

The Problem

$$i\hbar\partial_t|\psi\rangle = \hat{H}|\psi\rangle$$

The quantum state exists in an uncountably-infinite-dimensional Hilbert space.
Little intuition exists for reducing to a tractable subspace

Ehrenfest Theorem

$$\frac{d\langle\hat{A}\rangle}{dt} = \frac{i}{\hbar}\langle[\hat{H}, \hat{A}]\rangle + \left\langle\frac{\partial\hat{A}}{\partial t}\right\rangle$$

$$\begin{aligned}\frac{d\langle\hat{r}\rangle}{dt} &= \frac{\langle\hat{p}\rangle}{m_e} \\ \frac{d\langle\hat{p}\rangle}{dt} &= -\langle\nabla\hat{V}\rangle \\ &\vdots\end{aligned}$$

Approximations to the Schrödinger equation are equivalent to a closure in the evolution of the position-momentum moments

The Time Dependent Variational Principle

Time Dependent Variational Principle

$$\delta \int_{t_i}^{t_f} dt \langle \psi | i\partial_t - \hat{H} | \psi \rangle = 0$$

Feldmeier and Schnack (2000)

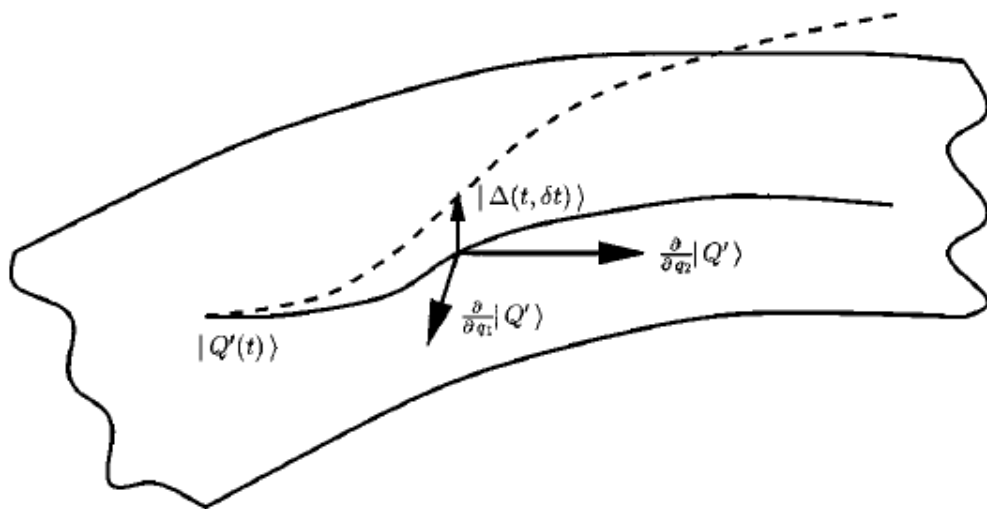


FIG. 1. Sketch of the manifold of trial states: solid line, the approximate time evolution; dashed line, the solution of the Schrödinger equation. The error $|\Delta(t, \delta t)\rangle$ is orthogonal to all tangent states $\partial/\partial q_\nu|Q'\rangle$.

What is the smallest subspace of the full Hilbert space which gives the right statistical properties (both static and dynamic)?

How can we balance accuracy and computational cost?

Wave Packet Molecular Dynamics

Variational Ansatz

Hartree Product (Slater Determinants can be used too)

Electron Coordinates

$$\psi(\vec{R}, t) = \prod_e \phi_e(\vec{r}_e, t) \quad \vec{R} = \{\vec{r}_1, \vec{r}_2, \dots, \vec{r}_{N_e}\}$$

Isotropic Gaussian

$$\phi_e(\vec{r}_e, t) = A(t) e^{-\alpha_e(t) |\vec{r}_e - \vec{x}_e(t)|^2 + i\vec{p}_e(t) \cdot (\vec{r}_e - \vec{x}_e(t))}$$

$$A(t) = \left(\frac{3}{2\pi\sigma_e(t)^2} \right)^{3/4} \quad \alpha_e(t) = \frac{3}{4\sigma_e(t)^2} + i \frac{p_{\sigma,e}}{2\sigma_e}$$

Physical interpretation of variational parameters

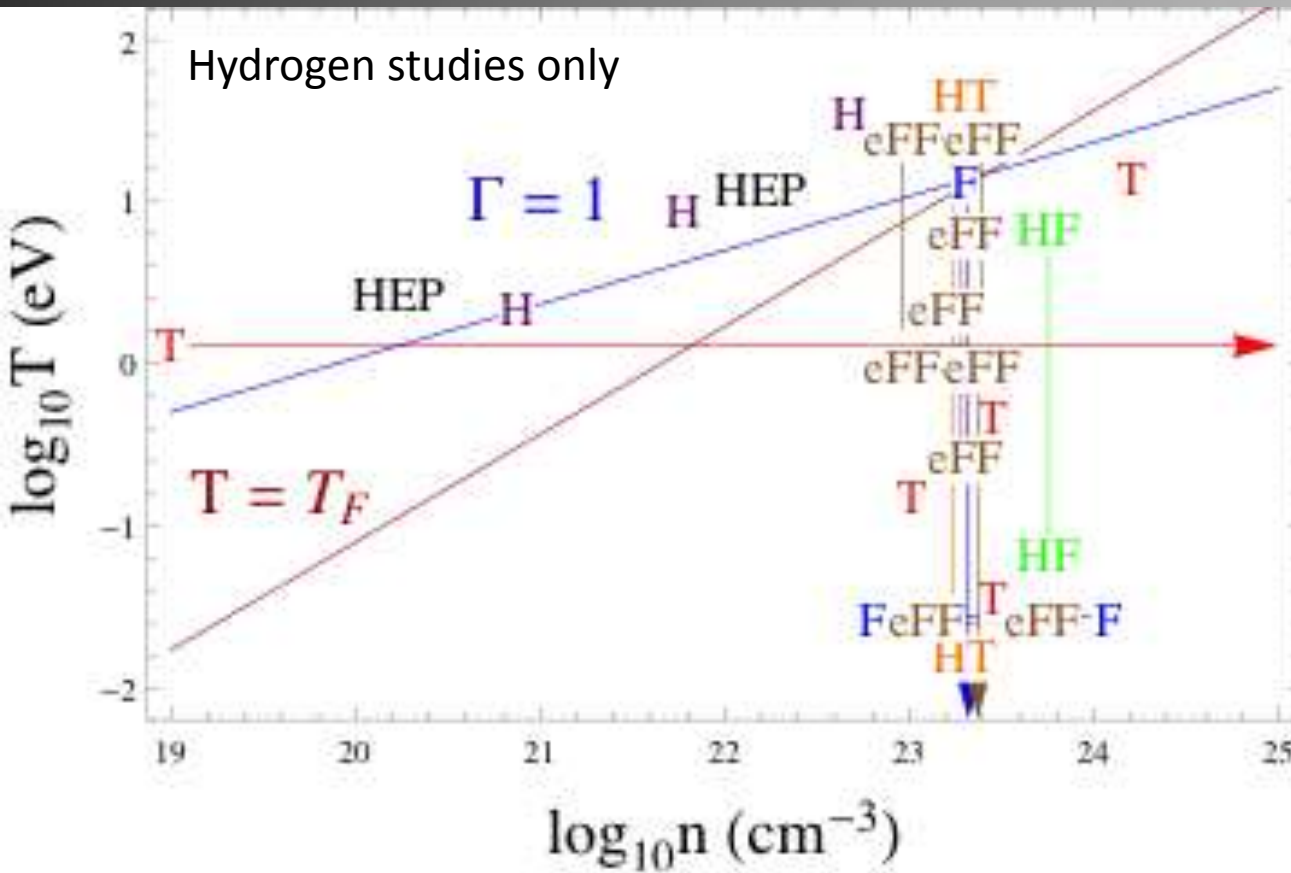
Classical-looking 4D Hamilton's equations

$$\begin{aligned} \langle \hat{\vec{r}}_e \rangle &= \vec{x}_e \\ \langle \hat{\vec{p}}_e \rangle &= \vec{p}_e \\ \langle \hat{r}_e^2 \rangle - \langle \hat{r} \rangle^2 &= \sigma_e^2 \\ \langle \hat{p}_e^2 \rangle - \langle \hat{p} \rangle^2 &= \frac{9}{4\sigma_e^2} + p_{\sigma,e}^2 \end{aligned}$$

$$\begin{pmatrix} \overleftarrow{0} & \overrightarrow{0} & -\overleftarrow{1} & \overrightarrow{0} \\ \overleftarrow{0} & 0 & \overleftarrow{0} & -1 \\ \overleftarrow{1} & \overrightarrow{0} & \overleftarrow{0} & \overrightarrow{0} \\ \overleftarrow{0} & 1 & \overleftarrow{0} & 0 \end{pmatrix} \begin{pmatrix} \dot{\vec{x}}_e \\ \dot{\sigma}_e \\ \dot{\vec{p}}_e \\ \dot{p}_{\sigma,e} \end{pmatrix} = \begin{pmatrix} \partial_{\vec{x}_e} \\ \partial_{\sigma_e} \\ \partial_{\vec{p}_e} \\ \partial_{p_{\sigma,e}} \end{pmatrix} \langle \hat{H} \rangle$$

Ions are treated completely classically

WPMD Simulations



Antisymmetrization Methods

T – Two-body antisymmetrization
 F – Full Antisymmetrization (with respect to kinetic energy only)
 eFF – Electron Force Field

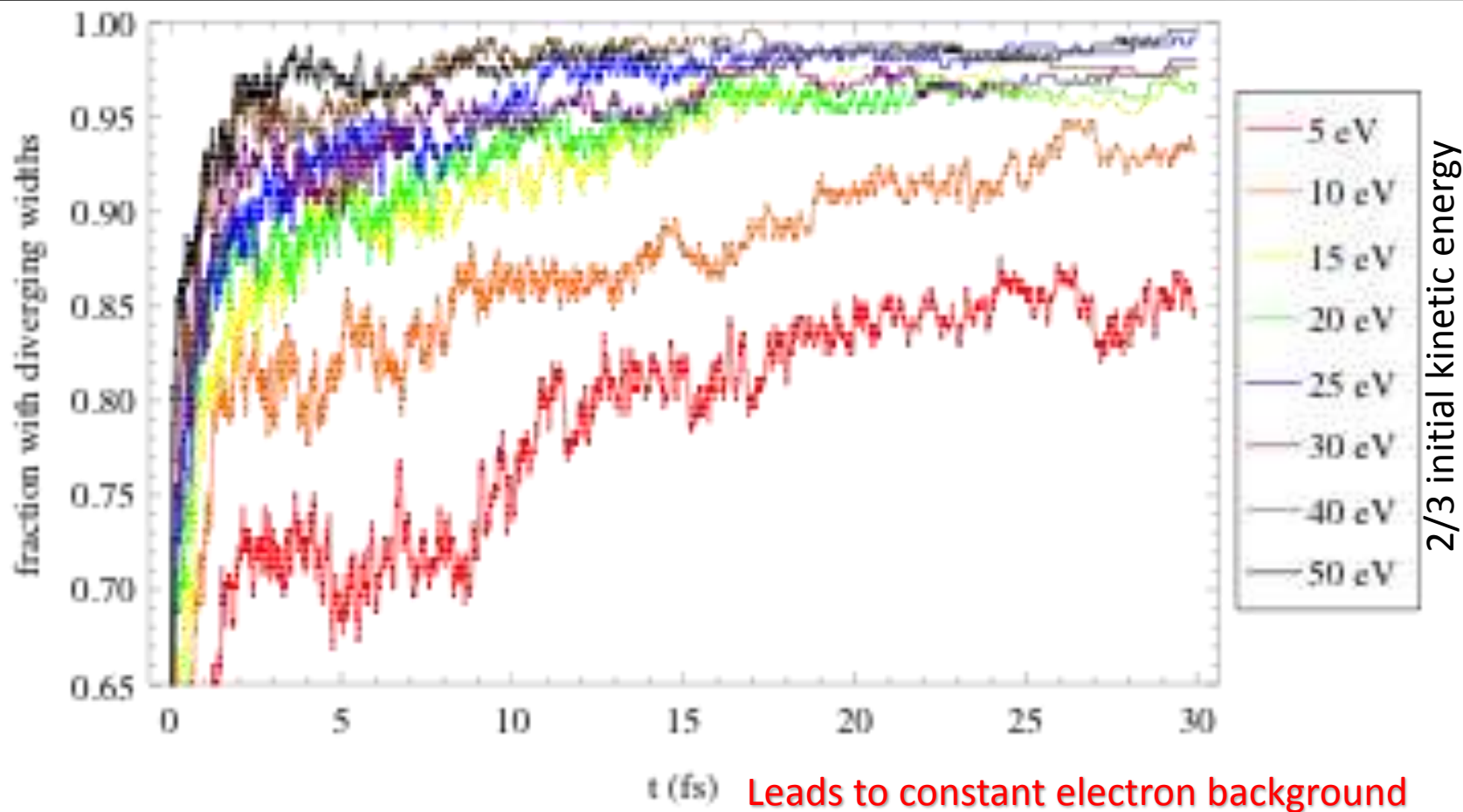
Width Constraint Methods

H – Harmonic Constraint
 E – Energy Constraint
 P – Periodic Boundary Condition Constraint

Ad hoc constraints are needed at high temperatures to get sensible answers.

Klakow et al. 1994a, Klakow et al. 1994b, Klakow et al. 1996, Knaup et al. 1999, Knaup et al. 2000, Knaup et al. 2001, Knaup et al. 2002, Knaup et al. 2003, Zwicky and Pschiwul 2006, Jakob et al. 2007, Su and Goddard 2007, Morozov and Valuev 2009, Jakob et al. 2009, Su and Goddard 2009, Jaramillo-Bolero et al. 2010

Wave Packet Spreading in Wave Packet Molecular Dynamics



Much of coding by Dave Richards

Width Constraints

Morozov and Valuev 2009

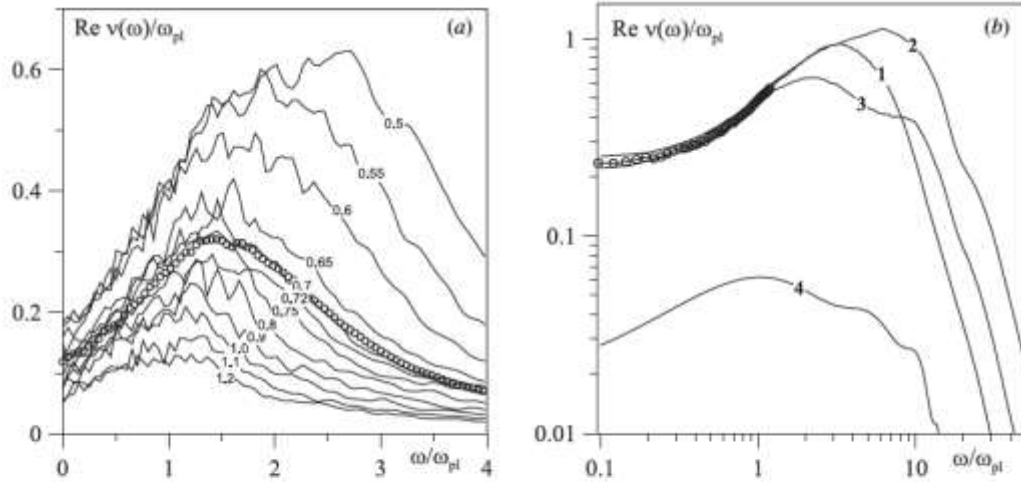


Figure 1. Real part of the dynamical collision rate. (a) Fitting of WPMD with the harmonic constraint (solid lines, values of γ_0/λ_{th} are shown on the curves) to the MD with the Kelbg potential (circles); $T = 1.35 \times 10^5$ K, $\Gamma = 1$. (b) 1 (circles): MD with the Kelbg potential, 2: WPMD with the harmonic constraint, $\gamma_0/\lambda_{th} = 0.88$, 3: WPMD with the energy-based constraint, $U_0/k_B T = 5$, 4: WPMD with PBS for WP widths; $T = 3 \times 10^4$ K, $\Gamma = 1$.

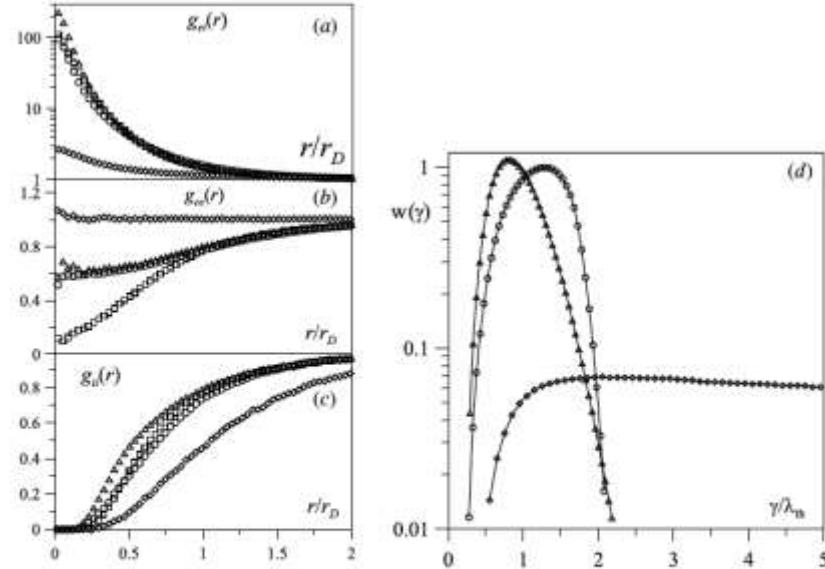


Figure 2. (a)–(c) Pair distributions and (d) the WP width distributions for MD with the Kelbg potential (squares, (a)–(c) only), WPMD with the harmonic constraint (triangles), WPMD with the energy-based constraint (circles), WPMD with the PBS for WP widths (rhombus). Simulation parameters are the same as in figure 1(b).

A change in variational ansatz

$$\phi_i = \left(\frac{3}{2\pi\beta_l}\right)^{3/4} \exp\left(-\left(\frac{3}{4\beta} + ip_\beta\right)(x_i - r_i)^2 + i\frac{d}{\beta}(x_i - r_i)^4 - ip_i(x_i - r_i)\right)$$

leads to a harmonic constraint on the width

$$H = \sum_i H_i + \sum_{i < j} V_{ij}, \quad H_i = \frac{p_i^2}{2m} + \frac{\hbar^2}{m} \left(\frac{9}{8\beta_i} + 2\beta_i p_{\beta_i}^2 + \frac{280}{9} d^2 \beta_i - \frac{40}{3} d\beta_i p_{\beta_i} \right)$$

Ebeling et al. 2006, width constraint first introduced by Knaup et al. 1999

Energy Constraint

$$\Delta H = A(\sigma(t) - \sigma(t_0))^6$$

Periodic Boundary Conditions

$$\sigma_{Max} = -\sigma_{Max}$$

Constraints lead to empirical parameters, and can get some physics right.

Electron Force Field Method

Su and Goddard 2007

Su and Goddard 2009

Jaramillo-Botero et al. 2011

$$E_{\text{Pauli}} = \sum_{\sigma_i = \sigma_j} E(\uparrow\uparrow)_{ij} + \sum_{\sigma_i \neq \sigma_j} E(\uparrow\downarrow)_{ij},$$

$$E(\uparrow\uparrow)_{ij} = \left(\frac{S_{ij}^2}{1 - S_{ij}^2} + (1 - \rho) \frac{S_{ij}^2}{1 + S_{ij}^2} \right) \Delta T_{ij}$$

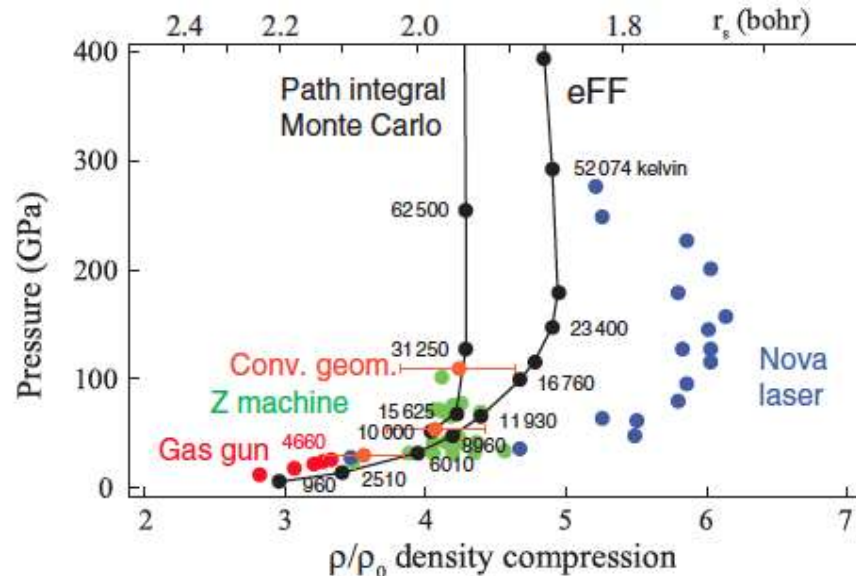
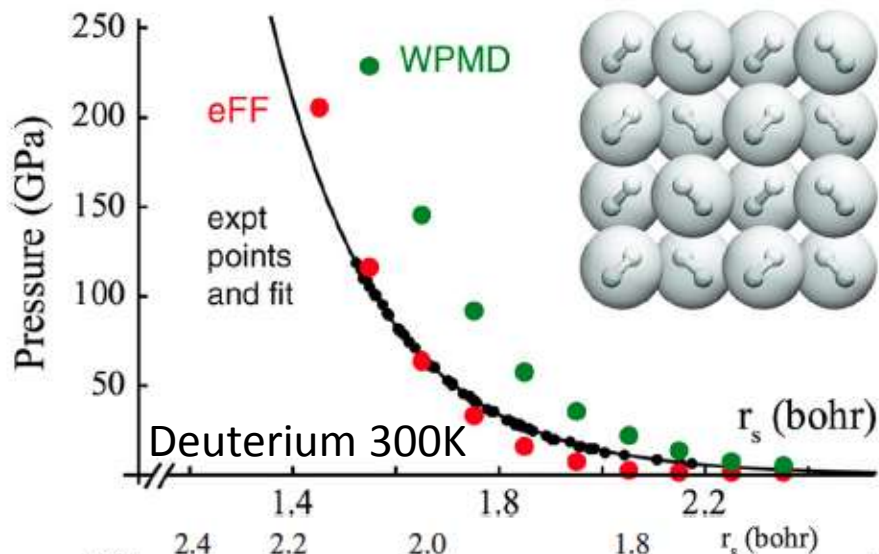
$$E(\uparrow\downarrow)_{ij} = \frac{\rho S_{ij}^2}{1 + S_{ij}^2} \Delta T_{ij}$$

$$\Delta T_{ij} = \frac{3}{2} \left(\frac{1}{\bar{s}_1^2} + \frac{1}{\bar{s}_2^2} \right) - \frac{2(3(\bar{s}_1^2 + \bar{s}_2^2) - 2\bar{x}_{12}^2)}{(\bar{s}_1^2 + \bar{s}_2^2)^2},$$

$$S_{ij} = \left(\frac{2}{\bar{s}_i/\bar{s}_j + \bar{s}_j/\bar{s}_i} \right)^{3/2} \exp(-\bar{x}_{ij}^2/(\bar{s}_i^2 + \bar{s}_j^2)),$$

Empirical parameters fixed by DFT calculations of molecules

$$\rho = -0.2, \quad \bar{x}_{ij} = x_{ij} \times 1.125, \quad \text{and} \quad \bar{s}_i = s_i \times 0.9.$$

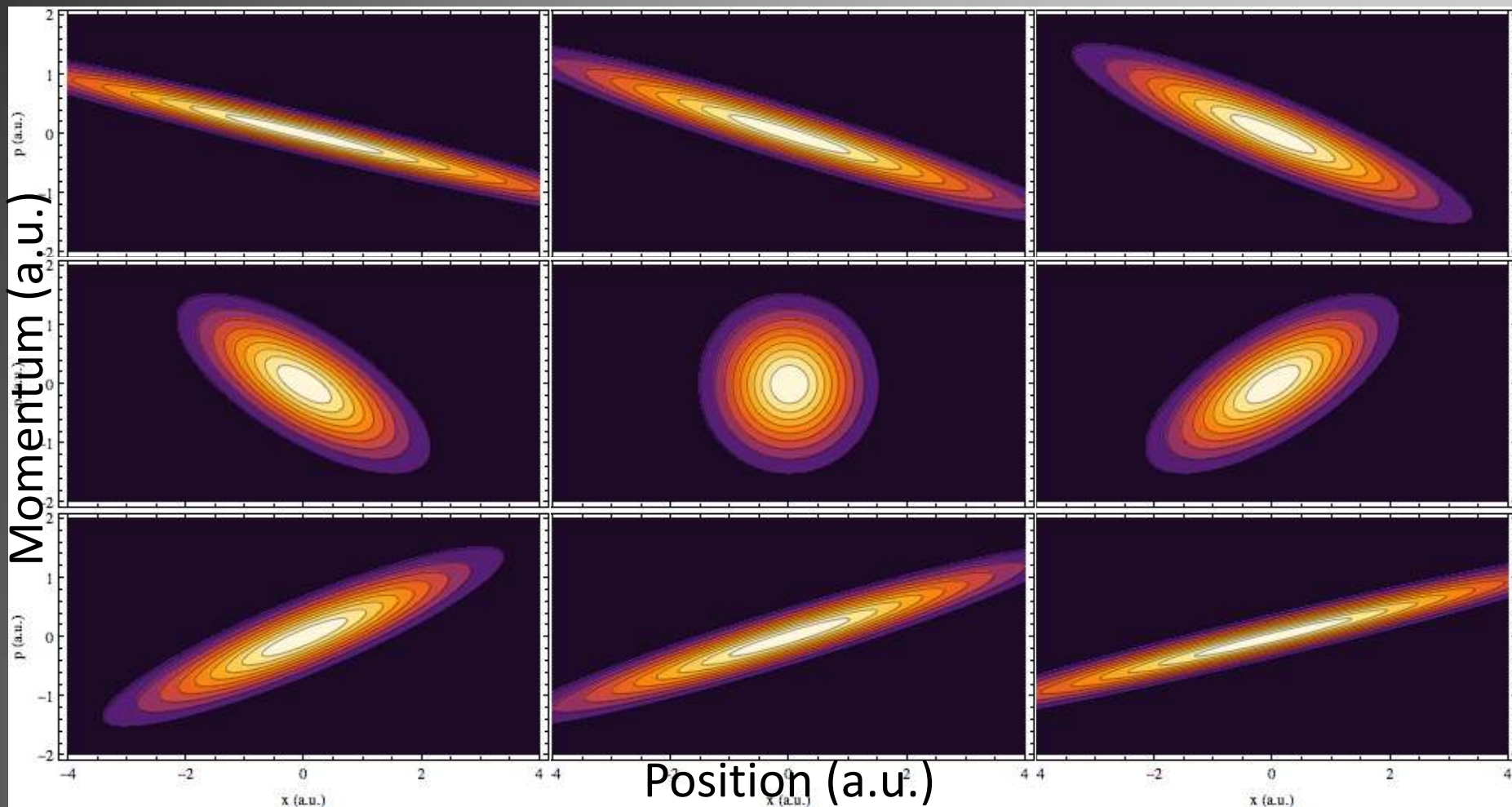


The Free Particle

Snapshots of Wigner phase space density of a single electron with $V=0$.

$\Delta t = 1 \text{ a.u.} \approx 0.024 \text{ fs}$

Wave packet spreading is a real physical phenomenon



Split Operator Fourier Transform

$$U(t, t + \Delta t) = e^{-i\hat{V}\frac{\Delta t}{2}} e^{-i\hat{T}\Delta t} e^{-i\hat{V}\frac{\Delta t}{2}} + \mathcal{O}[\Delta t^3]$$

Time dependent Schrödinger equation
solver on a Fourier grid (MxMxM).

$\Delta t = 10^{-4}$ fs
M = 128

**This method produces our
reference numerically exact
single particle solution**

Code and SOFT solution done by Andreas Markmann

Scattering from a Yukawa Field

$$n = 10^{24} \text{ cm}^{-3}$$

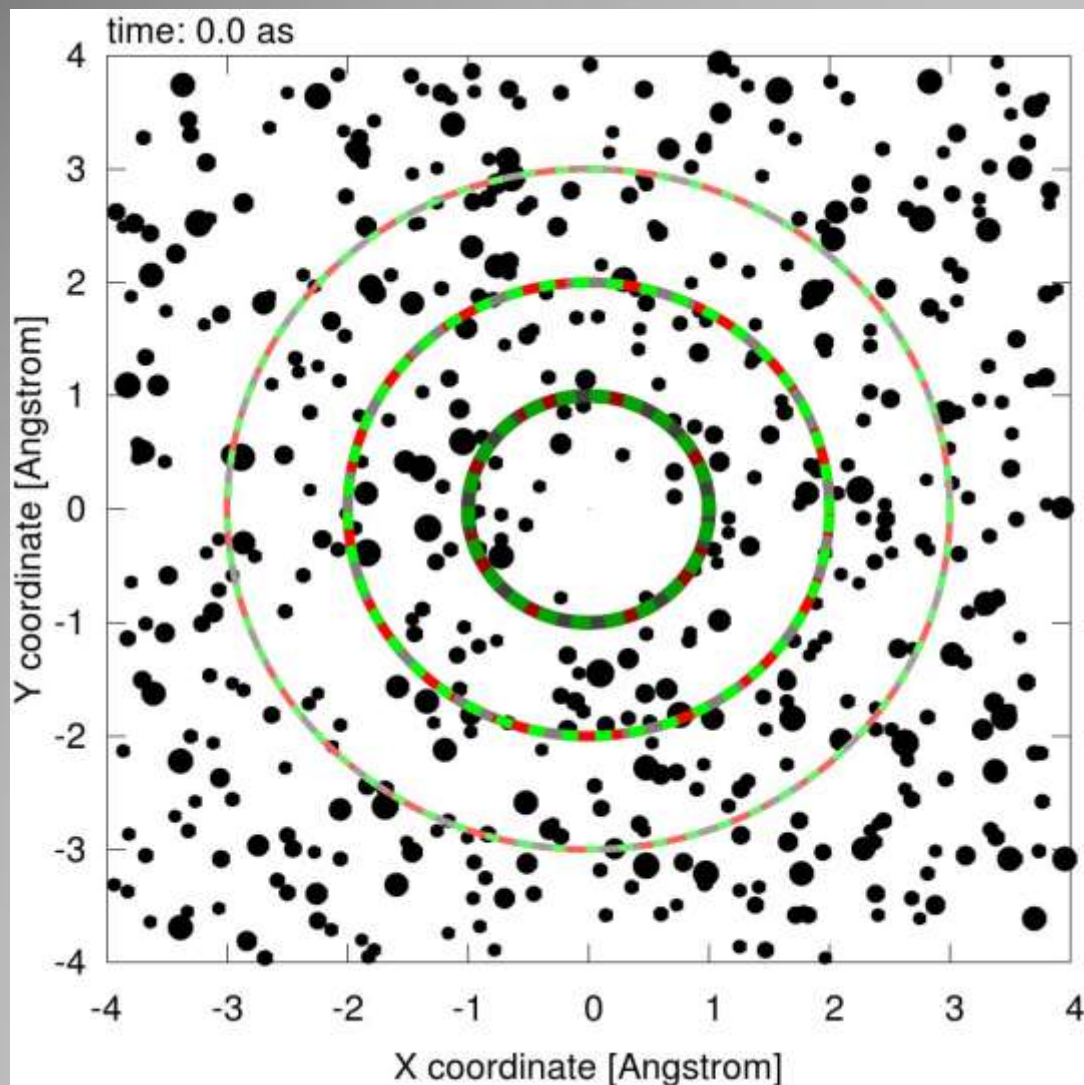
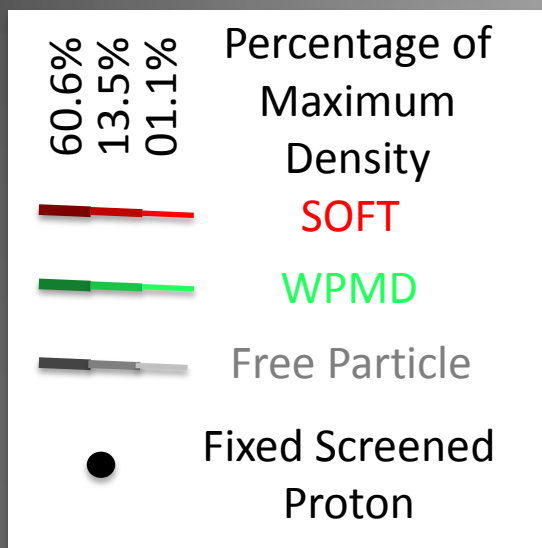
$$\frac{|\langle \hat{p} \rangle|^2}{2m_e} = 8.8 \text{ eV}$$

$$V(\vec{r}) = - \sum_{i=1, \vec{n}}^N \frac{e^{-r_{i\vec{n}}/\lambda}}{r_{i\vec{n}}}$$

$$r_{i\vec{n}} = |\vec{r} - \vec{R}_i - \vec{n}L|$$

$$N = 500$$

$$\lambda = 1 \text{ \AA}$$

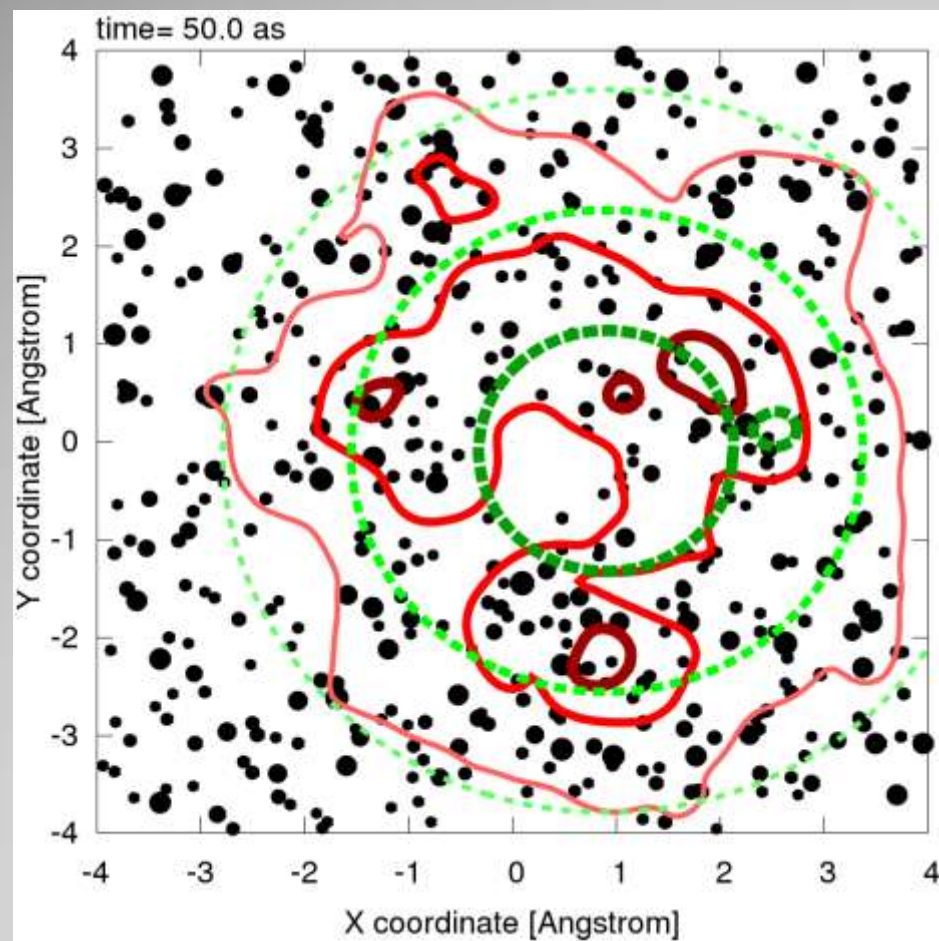
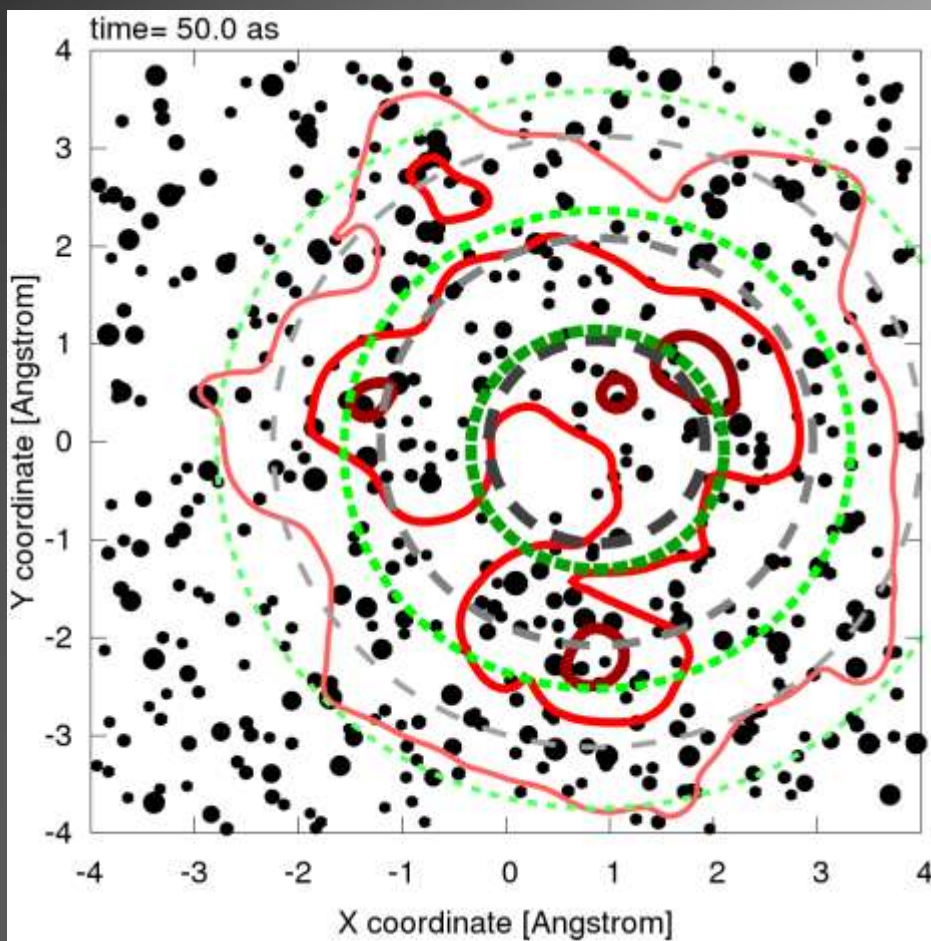


More Gaussians is Better

One Gaussian

See Ilya Valuev's poster or
Morozov and Valuev 2012

Two Gaussians

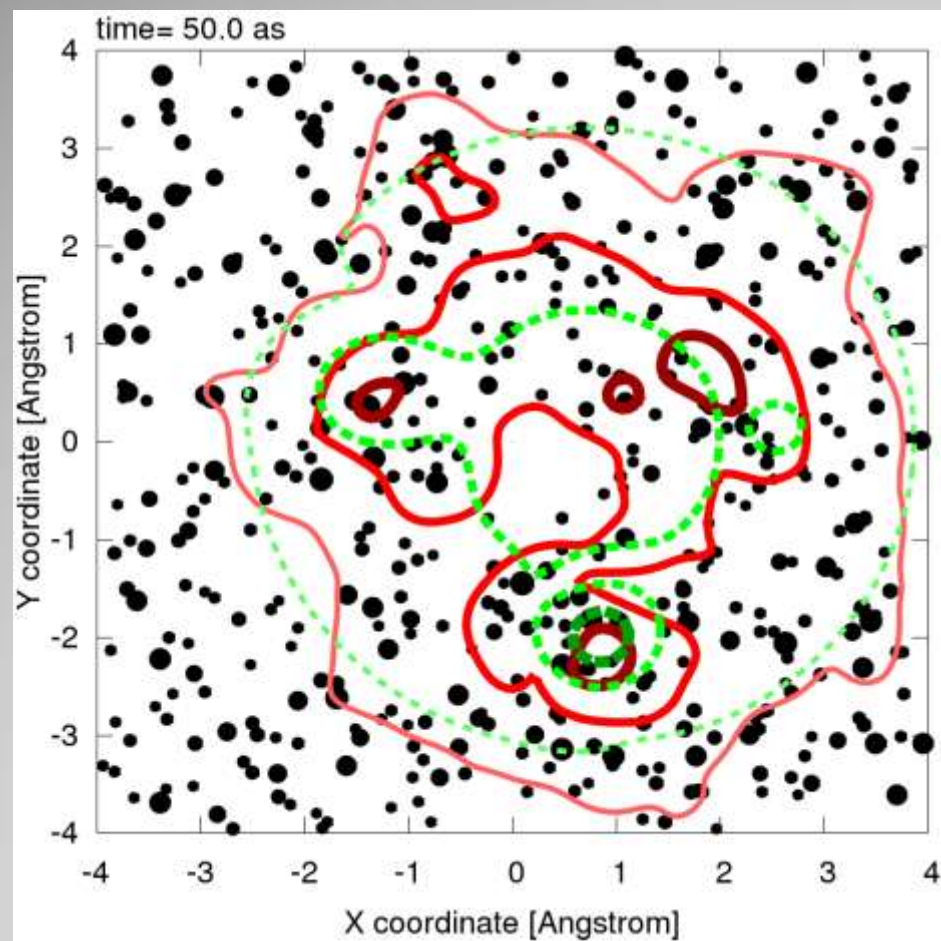
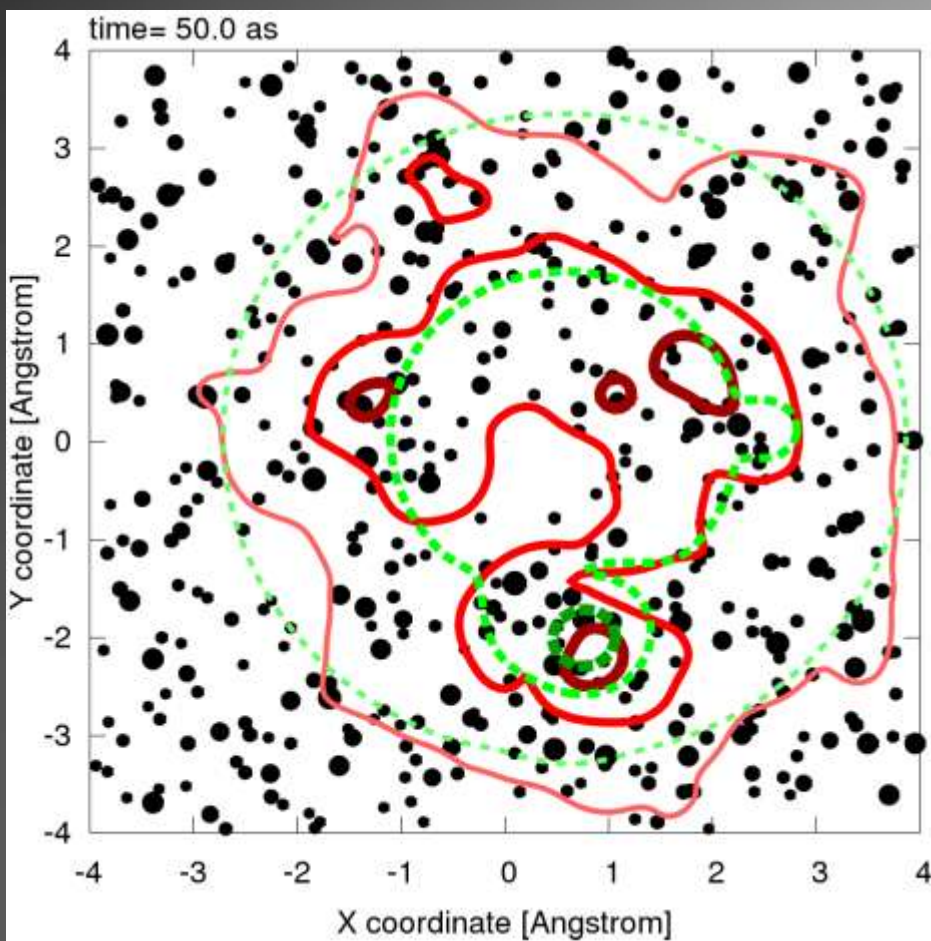


Courtesy of Ilya Valuev, Igor Morozov, and Andreas Markmann

More Gaussians is Better

Three Gaussians See Ilya Valuev's poster or
Morozov and Valuev 2012

Four Gaussians



Courtesy of Ilya Valuev, Igor Morozov, and Andreas Markmann

Localization from a Plane Wave

10 eV

$t = 0.05$ fs

85 eV

Probability isocontour
at four times average
density

High energy electrons
still prefer to be near ions
and do so despite having
large uncertainties in the
positions.

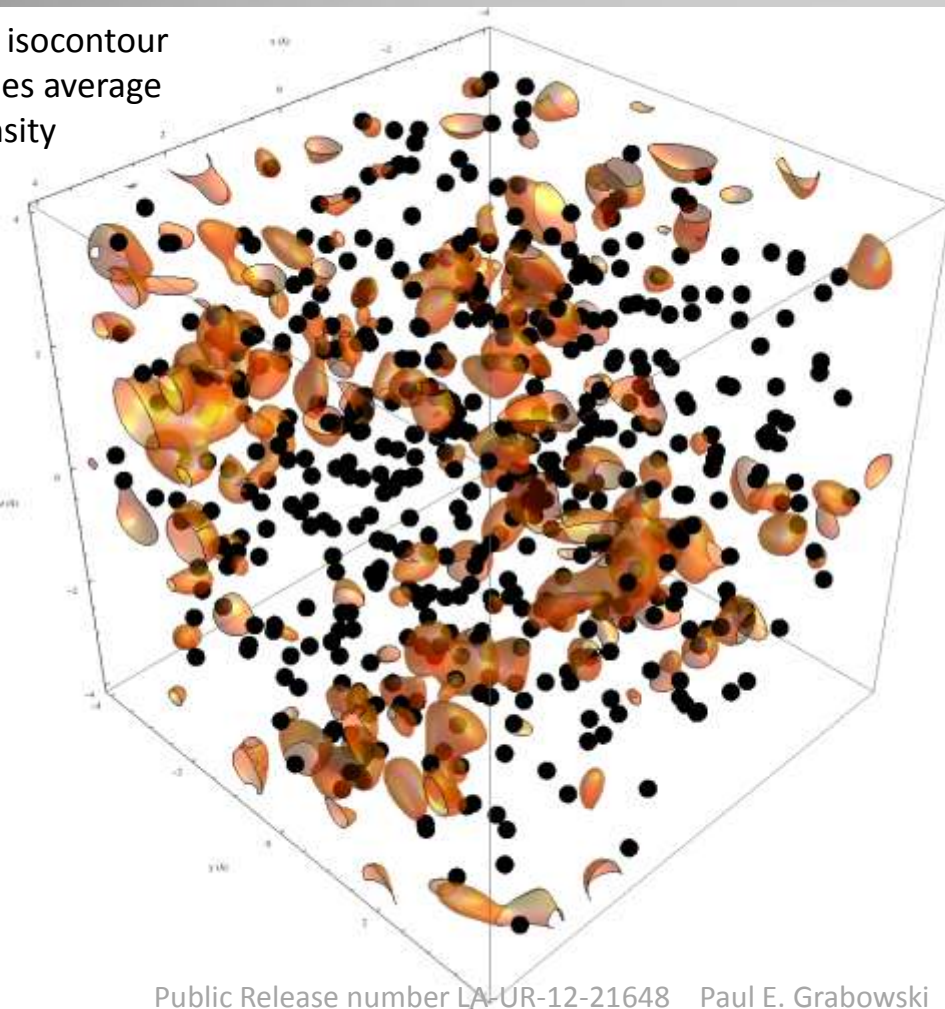
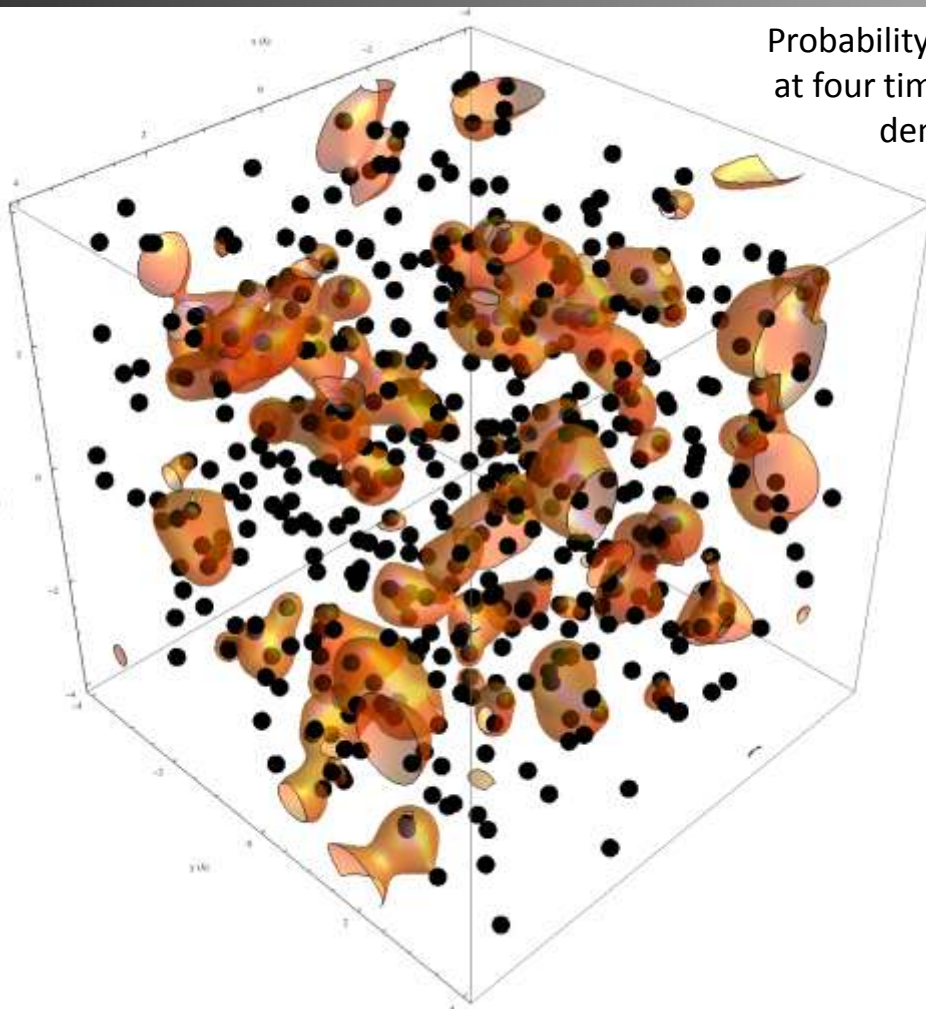
Localization from a Plane Wave

10 eV

$t = 0.10$ fs

85 eV

Probability isocontour
at four times average
density



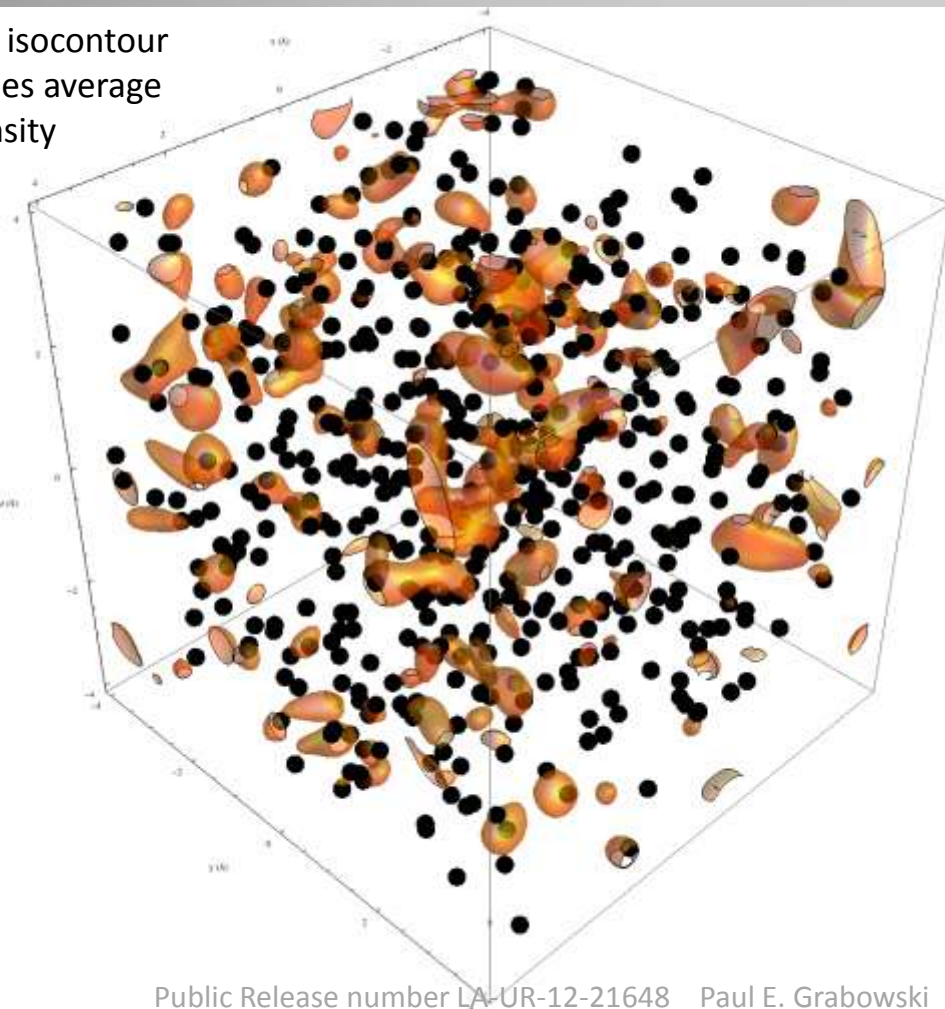
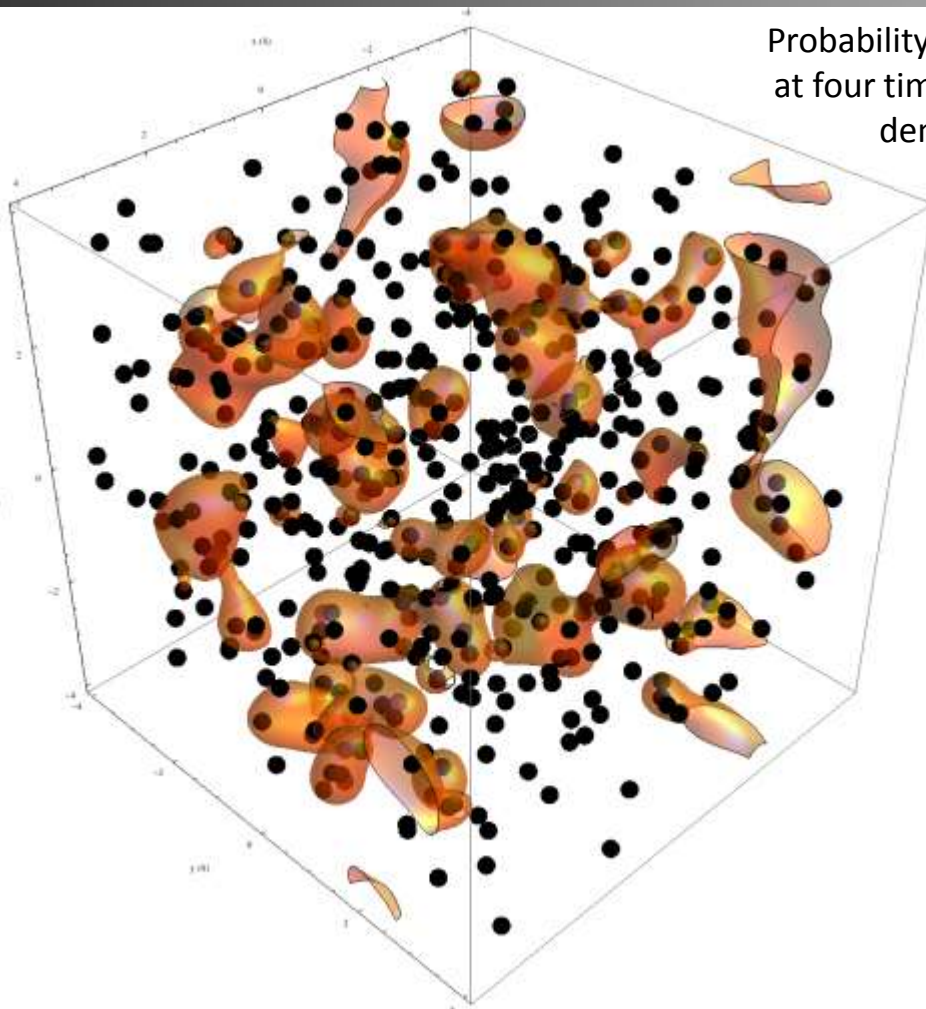
Localization from a Plane Wave

10 eV

$t = 0.15$ fs

85 eV

Probability isocontour
at four times average
density



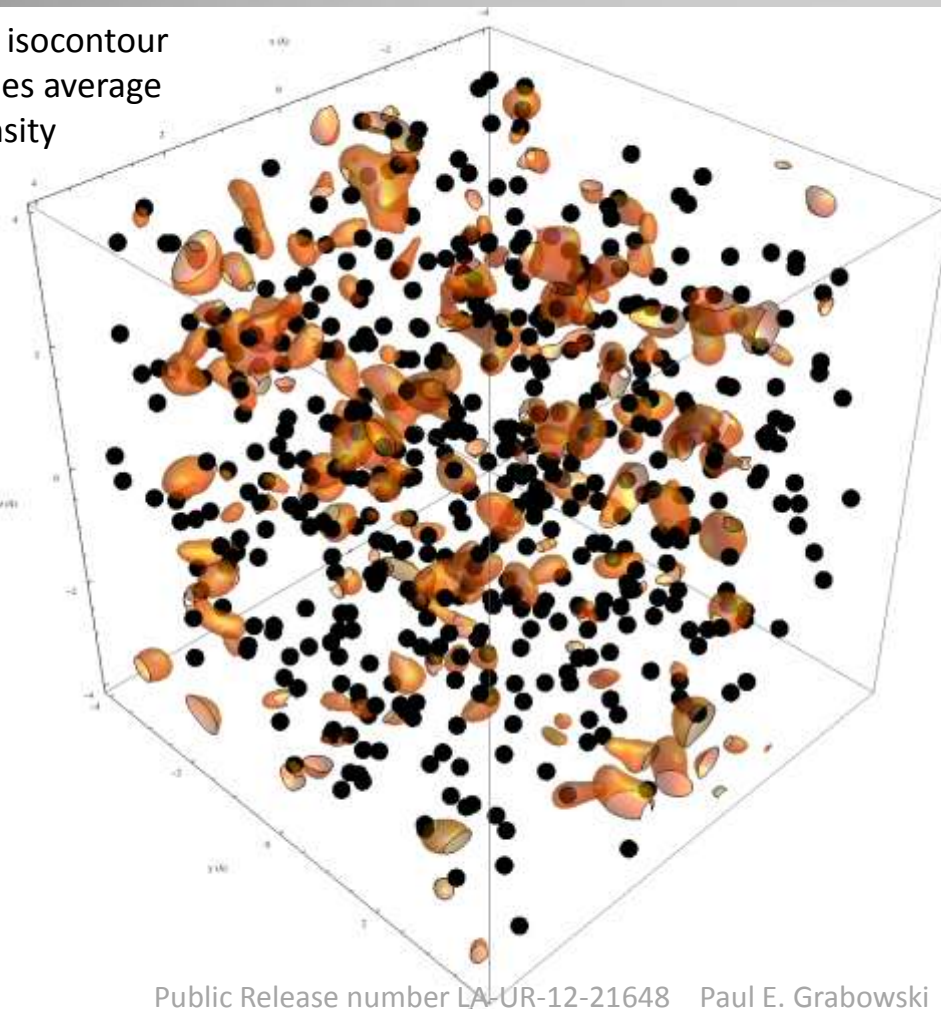
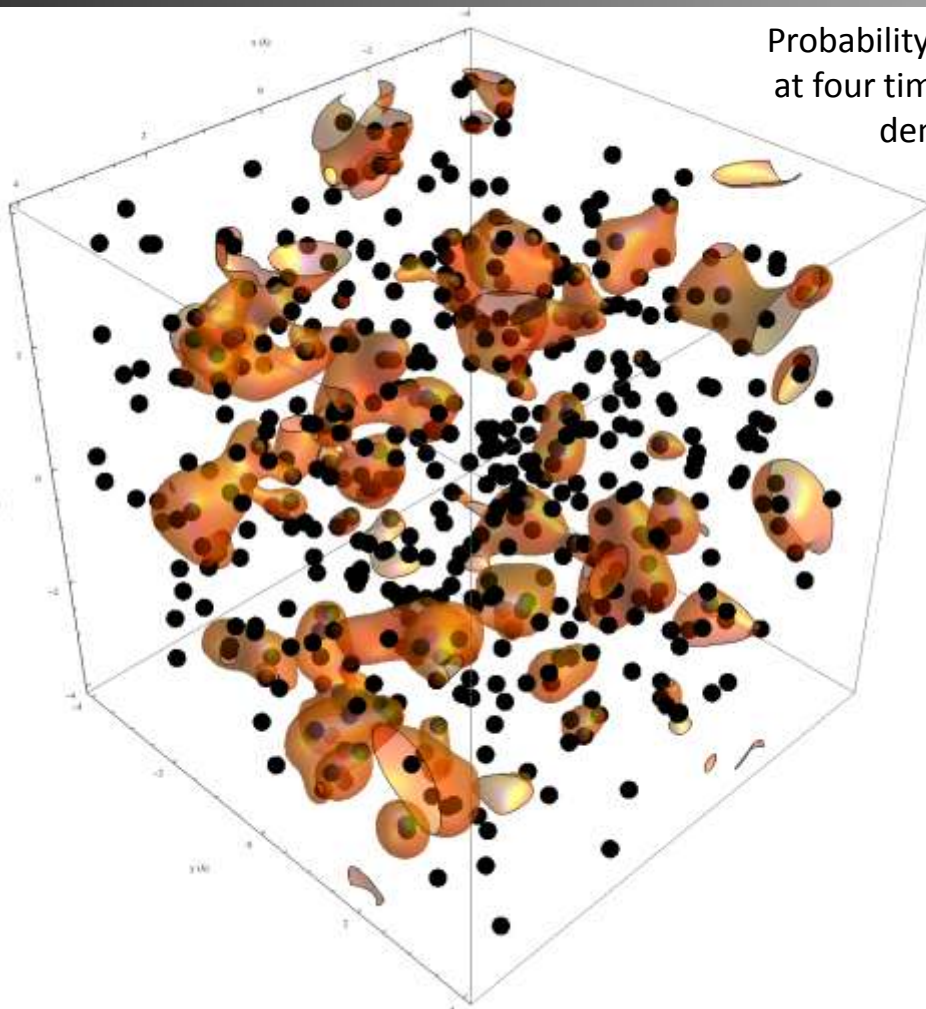
Localization from a Plane Wave

10 eV

$t = 0.20$ fs

85 eV

Probability isocontour
at four times average
density



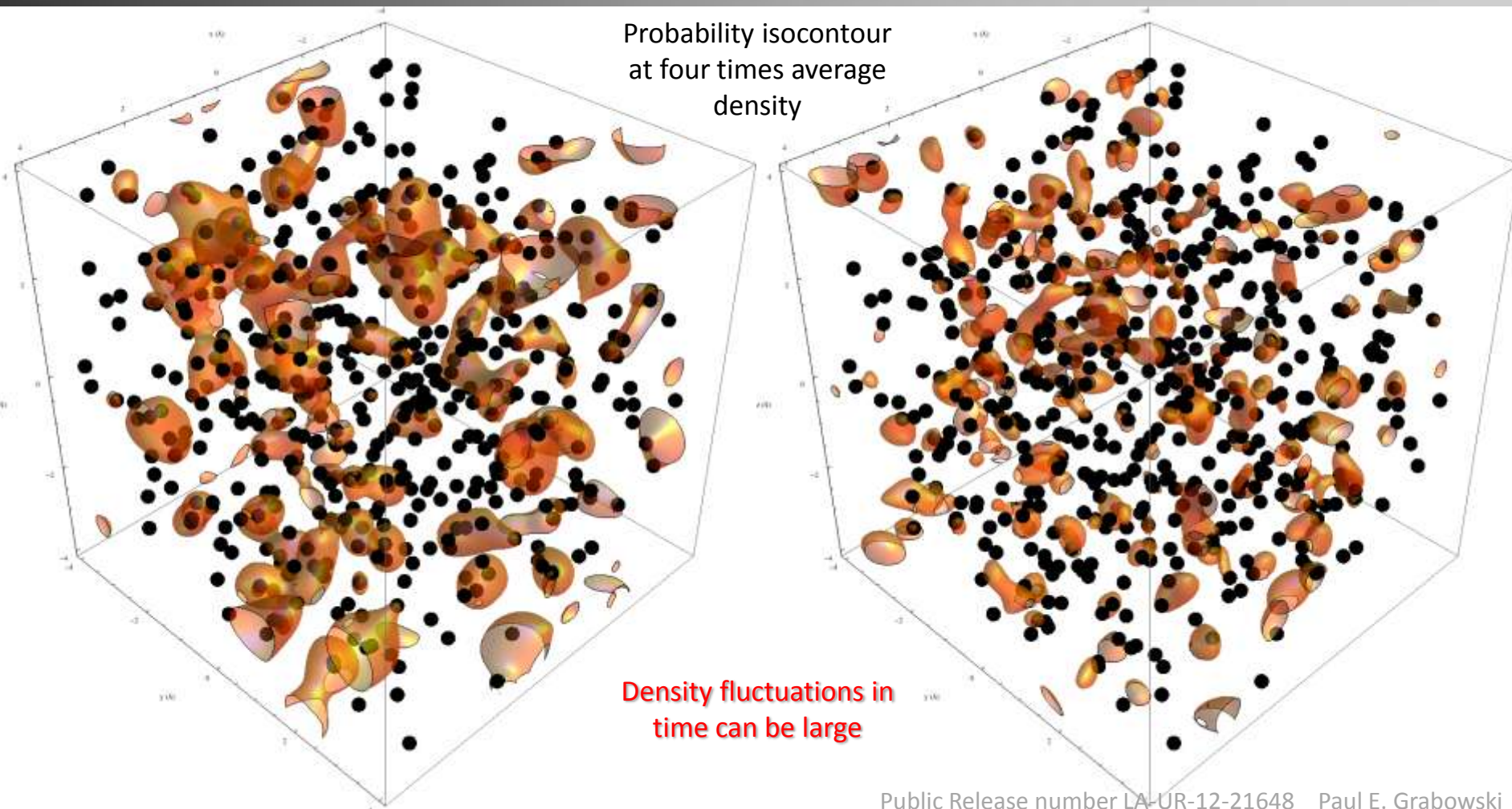
Localization from a Plane Wave

10 eV

$t = 0.25$ fs

85 eV

Probability isocontour
at four times average
density

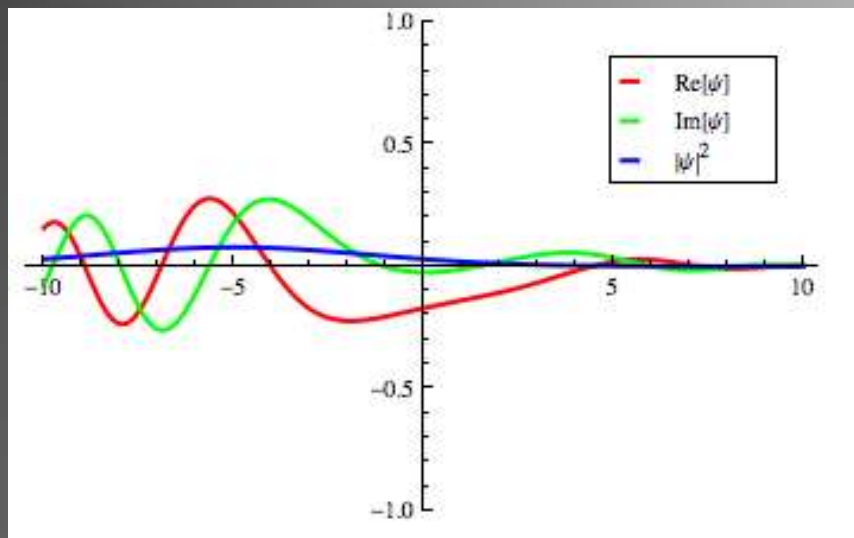


Density fluctuations in
time can be large

The Choice of Variational Ansatz

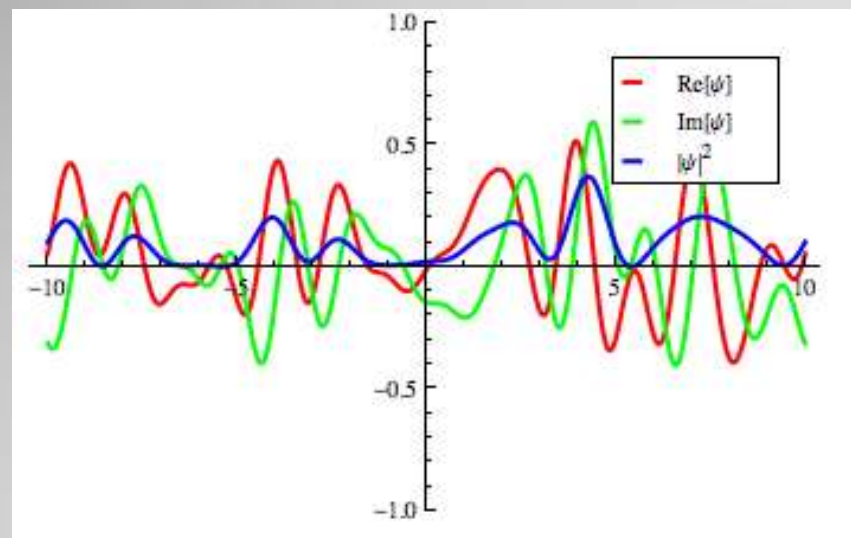
The Hartree approximation will be assumed here,
but at the expense of greater computation can be discarded

Wave Packet Ansatz



A Gaussian is limited to a very simple aperiodic form

Plane Wave Ansatz

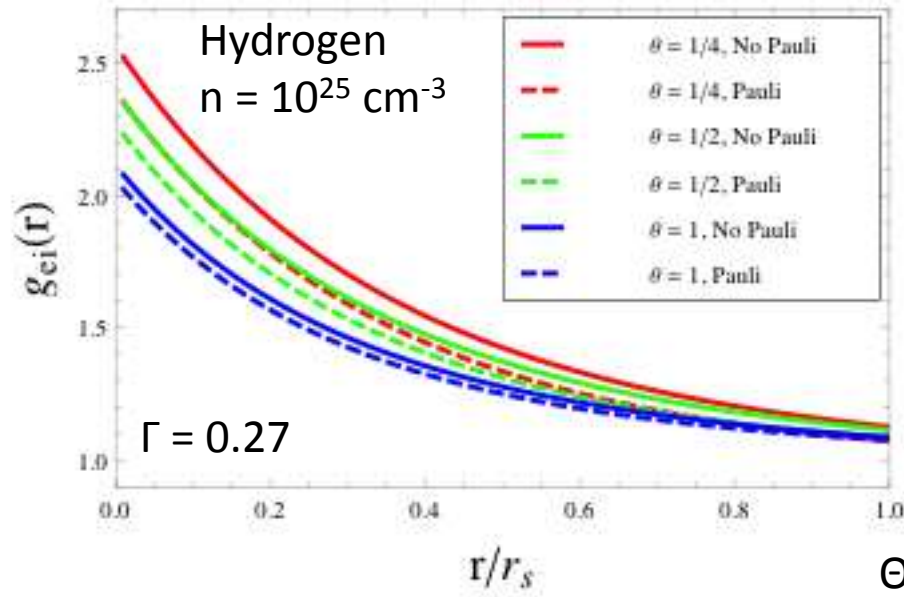


A full plane wave basis can represent any periodic function.

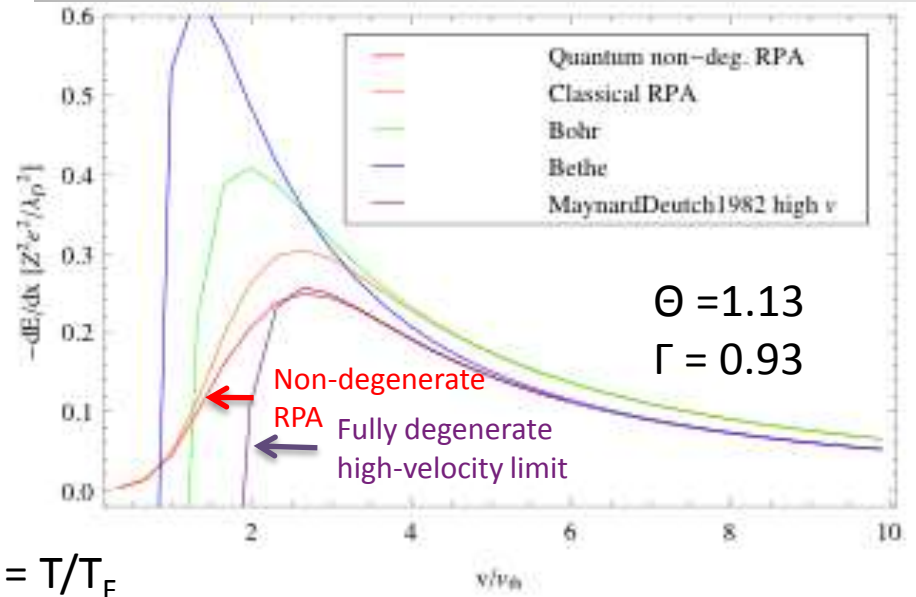
Philosophy

If one only cares about ion dynamics, one can hide all sorts of sins in the electron-electron interaction and still get dynamic electron screening right (at least at high temperature).

Radial Distribution Function



Stopping Power of a Proton by an Electron Target



Calculated with Hypernetted Chain using a Dunn-Broyles potential.

Degeneracy effects can often be small

Plane Wave Molecular Dynamics

Wave Function

$$\Psi(\vec{r}, t) = \frac{1}{V^{N/2}} \prod_e \phi_e(\vec{r}_e, t)$$

$$\phi_e(\vec{r}_e, t) = \sum_{\vec{k}} \phi_{e,\vec{k}}(t) e^{2\pi i \vec{k} \cdot \vec{r}_e / L}$$

$$\phi_{e,\vec{k}}(t) = q_{e,\vec{k}}(t) + i p_{e,\vec{k}}(t)$$

Equations of Motion

$$\dot{q}_{e,\vec{k}} = \frac{1}{2} \frac{\partial \langle \hat{H} \rangle}{\partial p_{e,\vec{k}}}$$

$$\dot{p}_{e,\vec{k}} = -\frac{1}{2} \frac{\partial \langle \hat{H} \rangle}{\partial q_{e,\vec{k}}}$$

$$\dot{\vec{R}}_i = \frac{\partial \langle \hat{H} \rangle}{\partial \vec{P}_i} \quad \dot{\vec{P}}_i = -\frac{\partial \langle \hat{H} \rangle}{\partial \vec{R}_i}$$

Scaling

$N =$ Number of particles

$M =$ Number of Fourier modes per dimension

$\mathcal{O}(NM^3)$ Memory

$\mathcal{O}(NM^3 \log M)$ Computation

Hamiltonian

$$\langle \hat{H} \rangle = T_i + V_{ii} + \langle \hat{T}_e \rangle + \langle \hat{V}_{ei} \rangle + \langle \hat{V}_{ee} \rangle \quad \langle \hat{T}_e \rangle = \frac{1}{2} \sum_{e,\vec{k}} k^2 |\phi_{e,\vec{k}}|^2$$

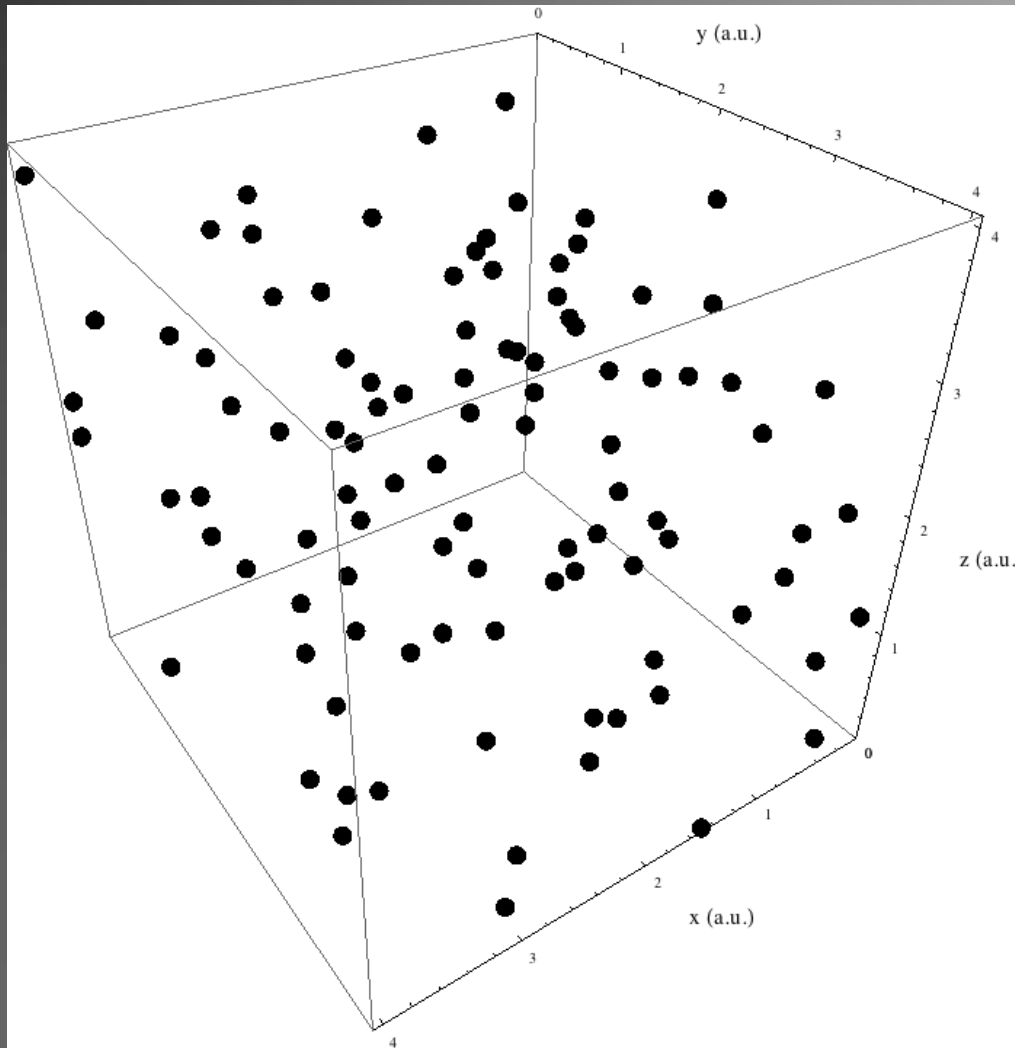
$$\langle \hat{V}_{ab} \rangle = \frac{1}{1 + \delta_{ab}} \sum_{\vec{n}} \int d^3 r_1 d^3 r_2 \frac{\left(\sum_{ij} \rho_{ai}(\vec{r}_1) \rho_{bj}(\vec{r}_2) \right) - \delta_{ab} \left(\sum_i \rho_{ai}(\vec{r}_1) \rho_{ai}(\vec{r}_2) \right)}{|\vec{r}_1 - \vec{r}_2 - \vec{n}L|}$$

Lattice Sum

Hartree Term

Self Energy

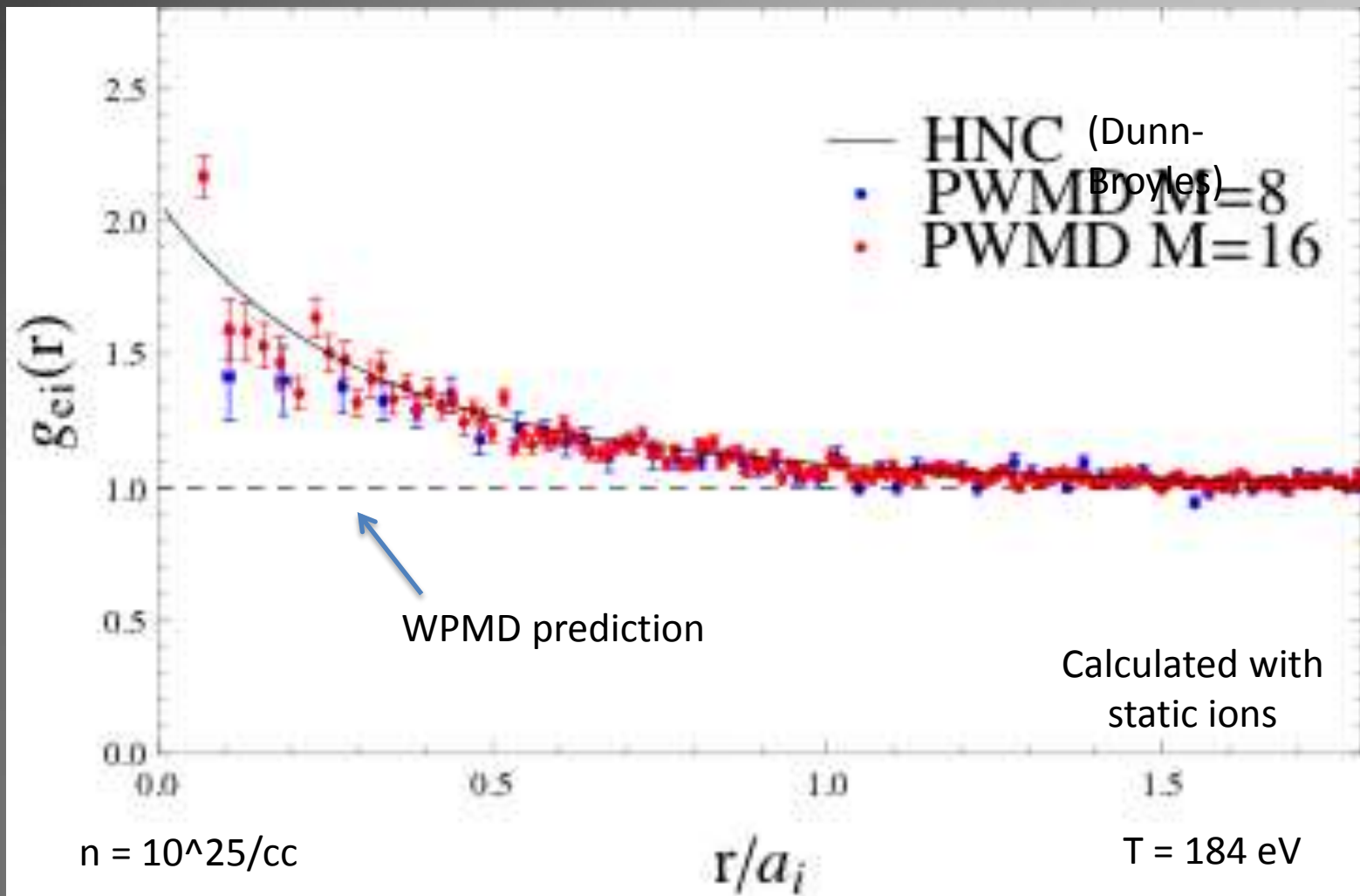
Plane Wave Molecular Dynamics Simulation



- Hydrogen Plasma
- $T = 184$ eV
- $n_{avg} = 10^{25}$ cm⁻³
- 100 protons and 100 electrons
- Black dots are protons
- Colors are electron density
- $M_p = 10m_e$
- Simulation time = 10a.u. = 0.24 fs
- Runs on my laptop overnight



Radial Distribution Function



Summary

- We have developed a quantum dynamic method
- The method is a good compromise between computational cost and accuracy
- We will now use it to calculate dynamic quantities (temperature relaxation, electrical conductivity, etc.)