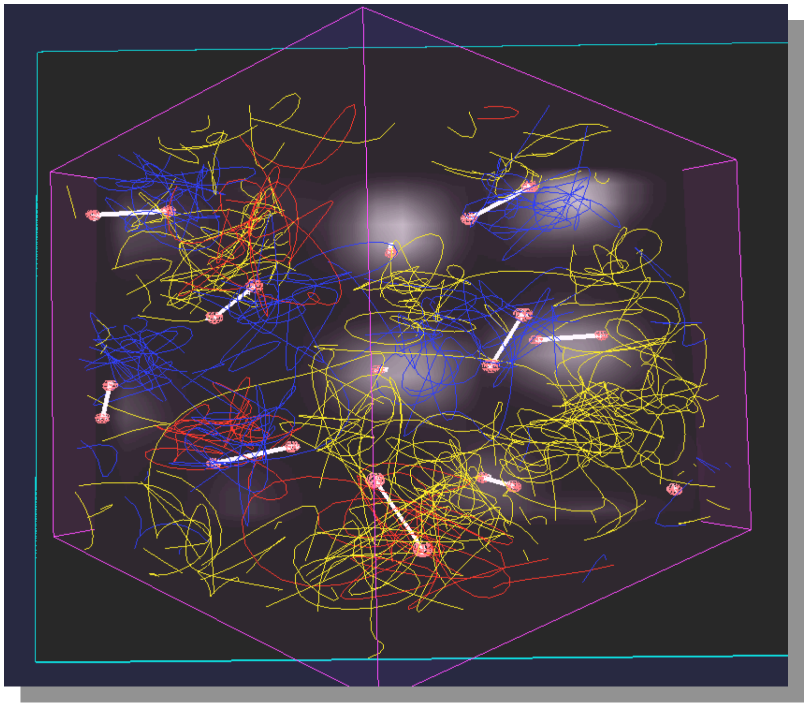
# QMC for Condensed Matter Systems at Finite Temperature




**Burkhard Militzer**

*January 24, 2006*

**Geophysical Laboratory**

*Carnegie Institution of Washington*


**http://militzer.gl.ciw.edu**

# Outline

1. Motivation for finite temperature quantum problem
   - Planetary applications

2. Path integral Monte Carlo for
   a) Distinguishable particles
   b) Bosons
   c) Fermions

3) Application to hot, dense hydrogen and helium, comparison with shock wave experiments

# Acknowledgements


## Hydrogen

**Path Integral Monte Carlo (PIMC)**

in collaboration with **D. Ceperley** (UIUC), **E.L. Pollock** (LLNL)

**Density Functional Theory**

**Jan Vorberger** (Carnegie, GL)

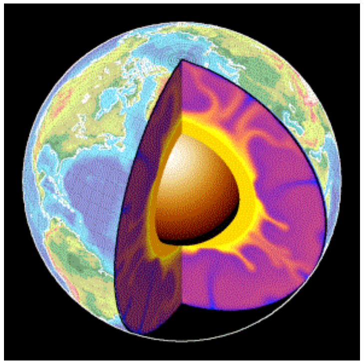
in collaboration with **S. Bonev, I. Tamblyn** (Dalhousie U.)

## Modeling Jovian planets

**W. Hubbard** (LPL)

**David Stevenson** (Caltech)

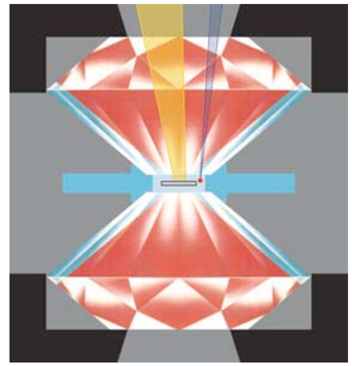
**Part of this work is supported by grants from NASA (PGG), NSF (AAG), and Carnegie Canada.**

Study earth materials

High pressure experiments

Now also astrobiology



Diamond anvil cell exp.:

Ho-kwang Mao,

Russell J. Hemley

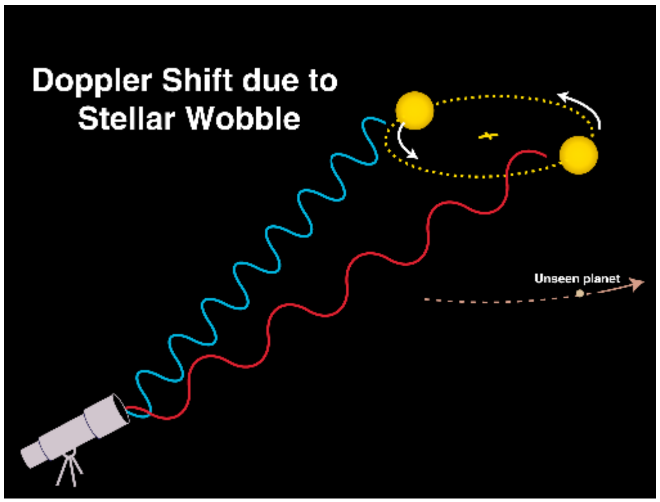

Original mission: Measure Earth's magnetic field (Carnegie ship)

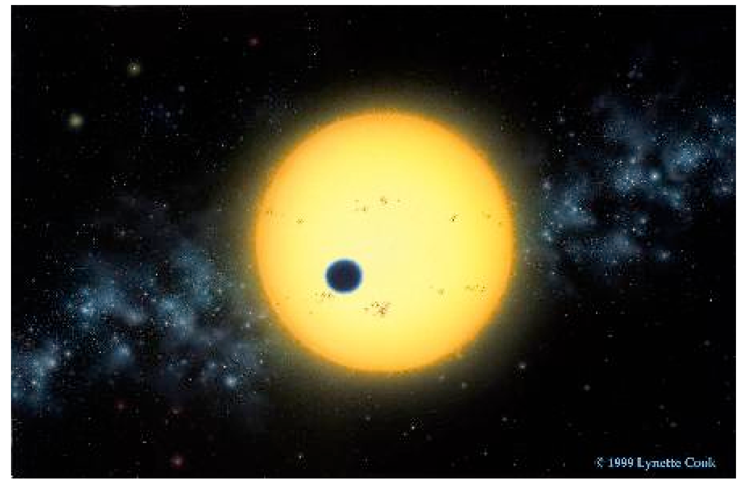
Today: astronomy (Vera Rubin, Paul Butler,…) and isotope geochemistry

**Postdoc fellowship program at GL (deadline Dec 31 annually):**

**`http://www.gl.ciw.edu`**

# Detection Techniques for Extrasolar Planets: Doppler shift vs. transient method

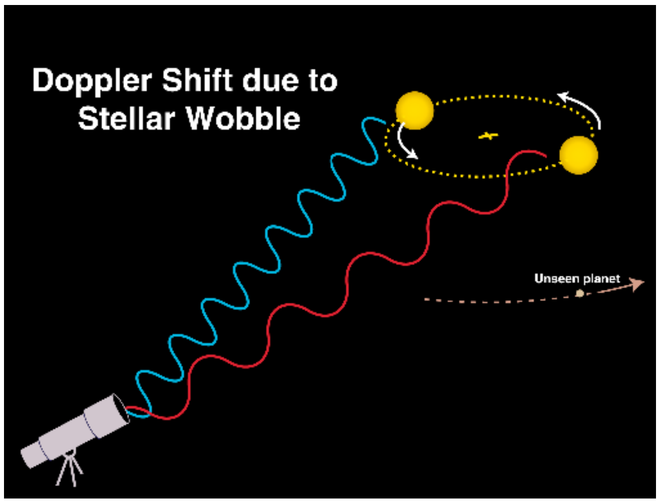


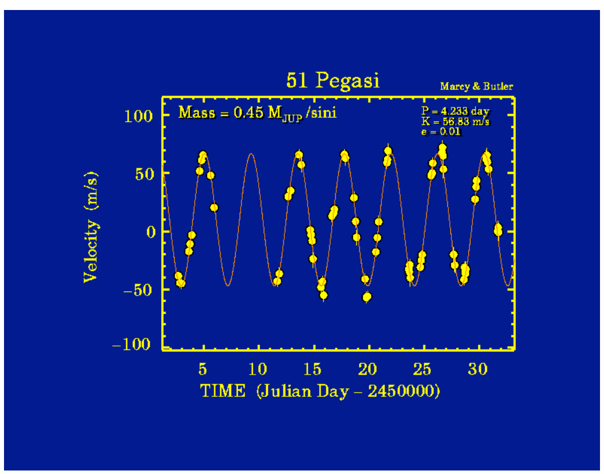




**Based on Jupiter's period of ~12 years Paul Butler at Carnegie started tiny frequency shift over longer time periods.**

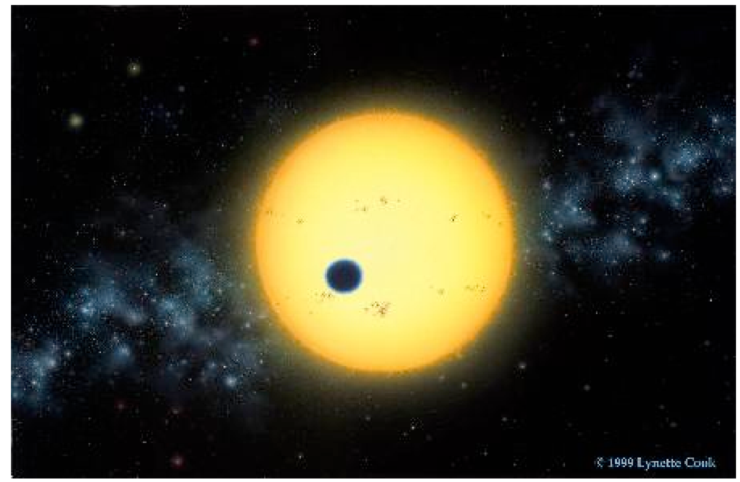
# Detection Techniques for Extrasolar Planets: Doppler shift vs. transient method

**168 planets found with Doppler method**




**10 planets seen with transient technique**



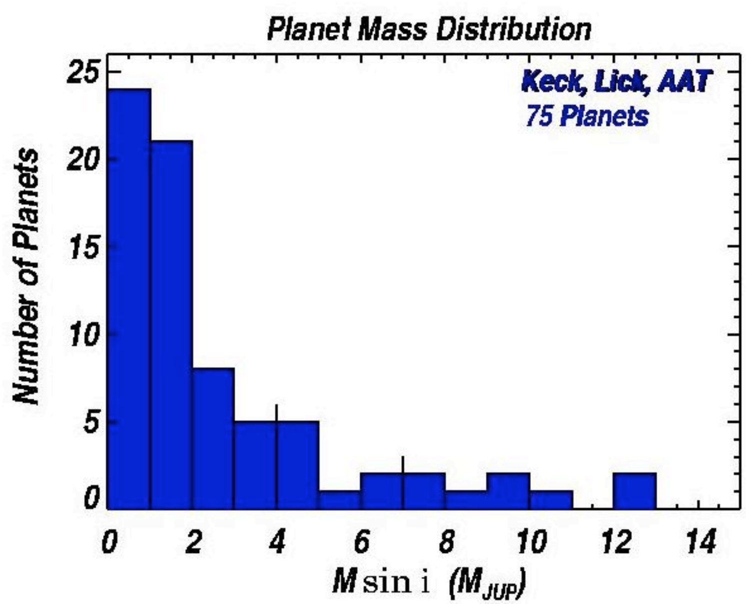

**First planet detected:**

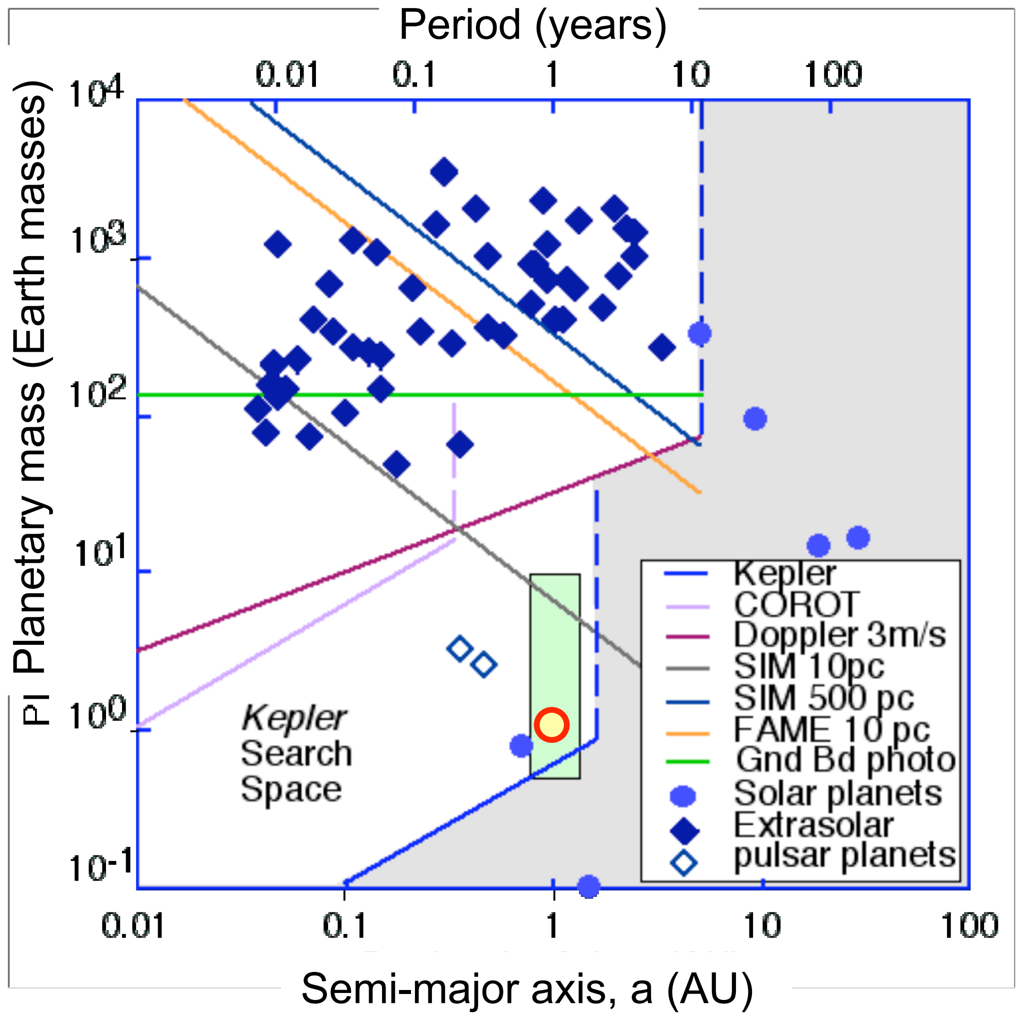
**Mayor & Queloz 1995, Nature 378, p. 355**
**(Geneva Observatory)**

Orbital period: 4.23 days !
Msin(i) = 0.46
a = 0.05 AU

# Characteristics of the ~168 known extrasolar planets

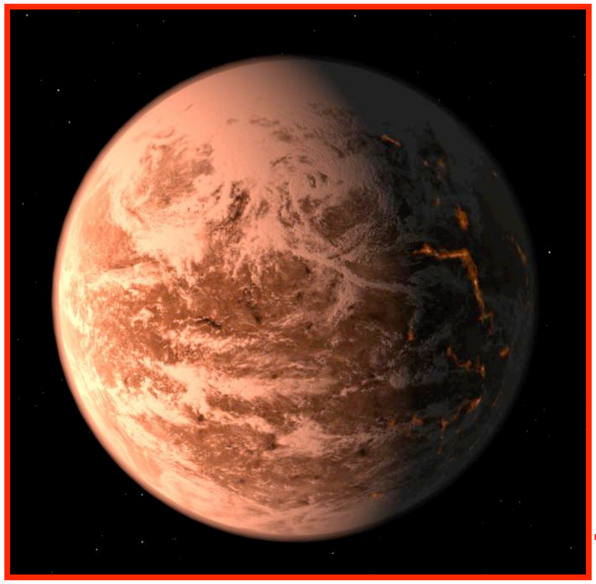
## How far away are we from detecting an Earth like planet?

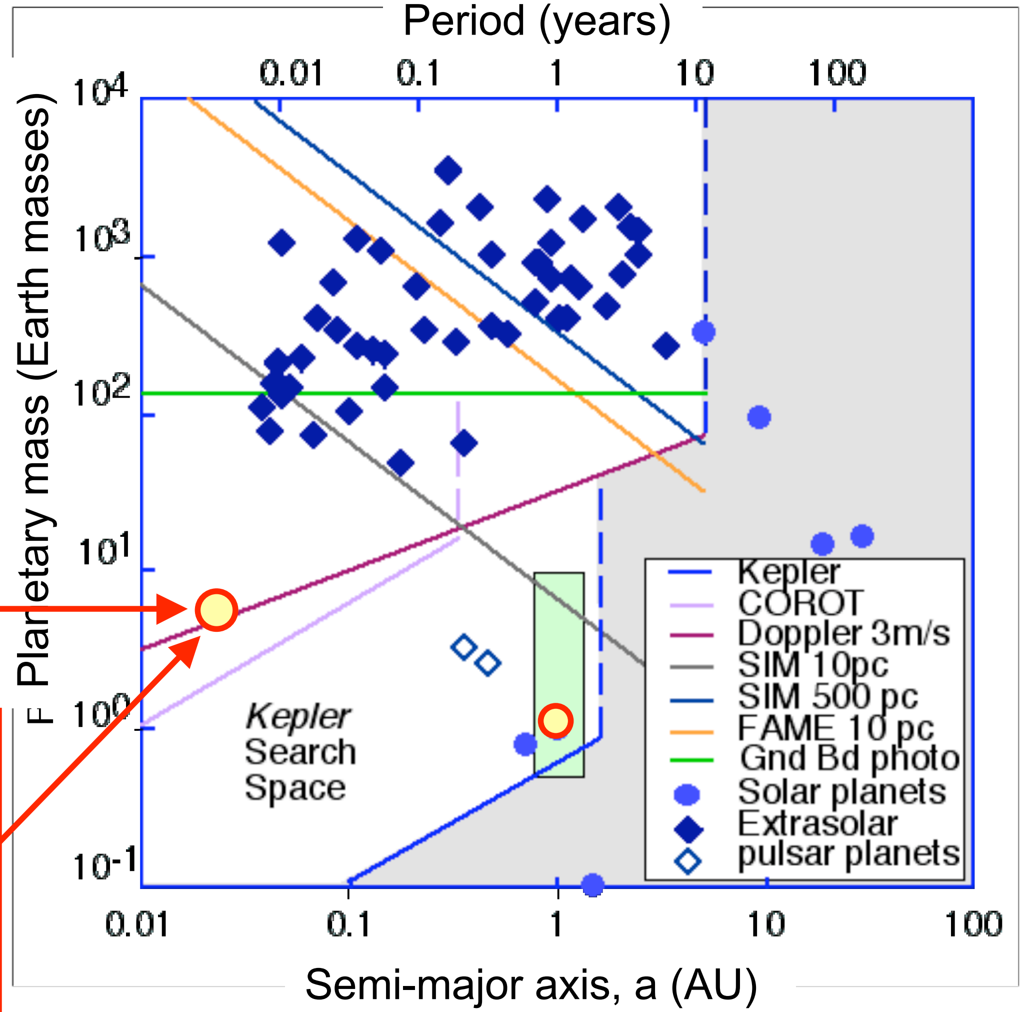


## Characteristics of the ~168 known extrasolar planets

## Recent light addition: a planet with only 6 Earth masses





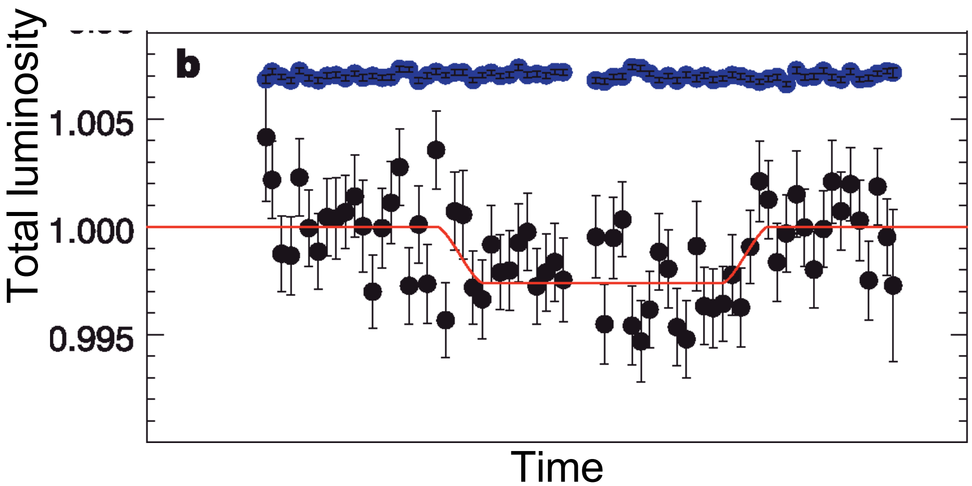

**Planet of 6-8 Earth-Masses Orbiting Close to Gliese 876**
**[E.Rivera, ApJ, in press]**

Orbital period: 1.94 days !

Msin(i) = 5.9 Earth masses

a = 0.021 AU

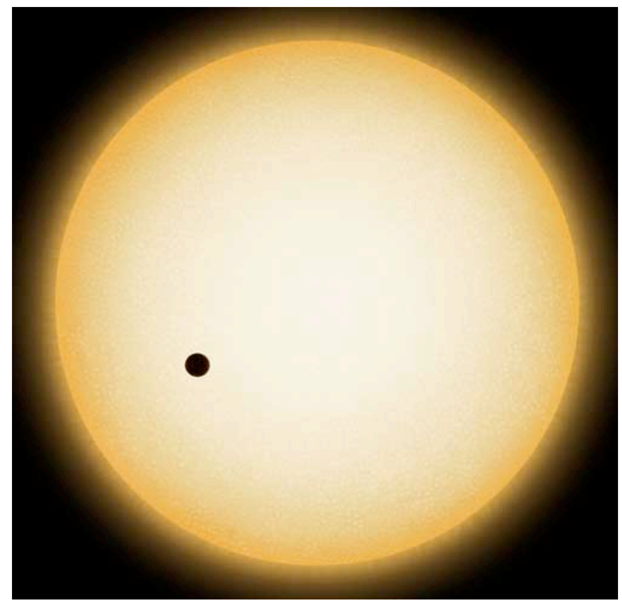
# Two very recent discoveries: 1) First observation of secondary eclipse 2) new transiting planet



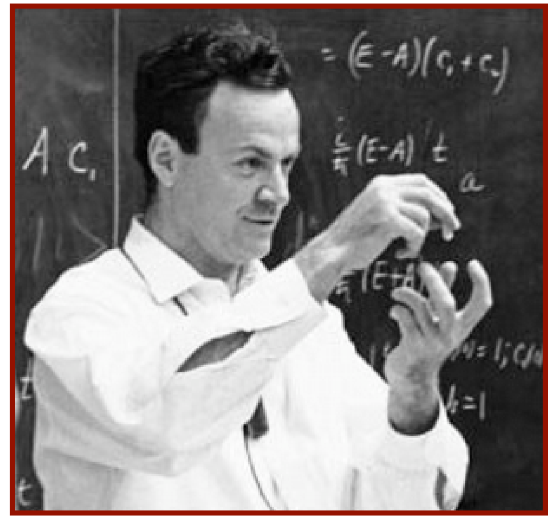

**1) First observation of a secondary eclipse of a extrasolar plant:**
Deming Nature 434 (2005) 740.
Charbonneau *et al.* Astrophys. J. (2005)

"Missing" light from planet can be characterized. Information about surface temperature and possibly composition.

**Saturn-mass planet with large dense core transits across HD 149026 [B. Sato et al. ApJ, in press].**



# Quantum systems at finite temperature: Richard Feynman's path integrals

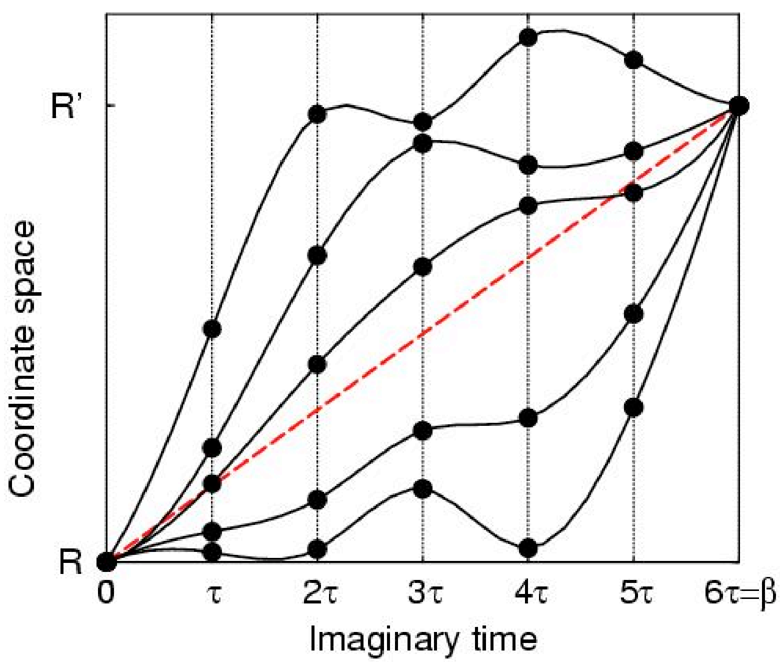


## Real time path integrals

**(not practical for simulations because oscillating phase)**

$$\Psi(R,t) = \int dR' \, G(R,R',t-t') \, \Psi(R',t')$$

$$\Psi(R,t) = \int dR' \, e^{-i(t-t')\hat{H}} \, \Psi(R',t')$$




## Imaginary time path integrals $\tau = it$

**(used for many simulations at T=0 and T>0)**

$$f(R,\tau) = \int dR' \, e^{-(\tau-\tau')\hat{H}} f(R',\tau')$$

$$\rho(R,R';\beta) = \langle R | e^{-\beta \hat{H}} | R' \rangle$$

$$e^{-\beta \hat{H}} = e^{-E / k_B T}$$

# Basic object for finite T QMC: Thermal density matrix $\rho(R,R';\beta)$

Density matrix definition:

$$\hat{\rho}(R,R';\beta) = \langle R | e^{-\beta \hat{H}} | R' \rangle$$

$$\hat{\rho}(R,R';\beta) = \sum_S e^{-\beta E_S}\ \psi_S^*(R)\ \psi_S(R')$$

Free particle density matrix:

$$\hat{\rho}(r,r';\beta) = (4\pi\lambda\beta)^{-D/2}\ \exp\left(-\frac{(r-r')^2}{4\lambda\beta}\right)$$

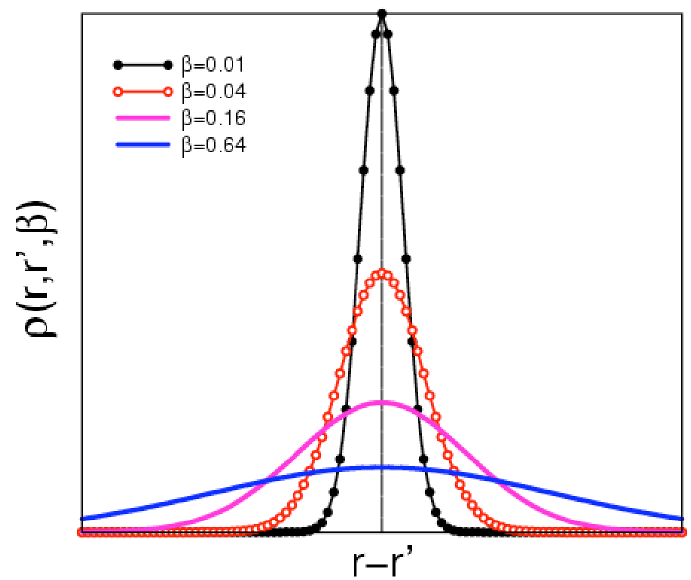
Density matrix properties:

$$Tr[\hat{\rho}] = \int dR\ \langle R | e^{-\beta \hat{H}} | R \rangle$$

$$\langle \hat{O} \rangle = \sum_S e^{-\beta E_S}\ \langle \psi_S | \hat{O} | \psi_S \rangle \Big/ Tr[\hat{\rho}]$$

$$\langle \hat{O} \rangle = \int dR\ \langle R | \hat{O}\, e^{-\beta \hat{H}} | R \rangle \Big/ Tr[\hat{\rho}]$$

$$\langle \hat{O} \rangle = Tr[\hat{O}\,\hat{\rho}] \Big/ Tr[\hat{\rho}]$$



# Path Integrals in Imaginary Time

**Every particle is represented by a path, a ring polymer.**

Density matrix: $\hat{\rho} = e^{-\beta \hat{H}} = \left( e^{-\tau \hat{H}} \right)^M \,, \quad \beta = \frac{1}{k_B T} \,, \quad \tau = \frac{\beta}{M}$

$$\langle \hat{O} \rangle = \frac{\mathrm{Tr}[\hat{O}\hat{\rho}]}{\mathrm{Tr}[\hat{\rho}]}$$

Trotter break-up:

$$\langle R | \hat{\rho} | R' \rangle = \langle R | (e^{-\tau \hat{H}})^M | R' \rangle = \int dR_1 \ldots \int dR_{M-1} \langle R | e^{-\tau \hat{H}} | R_1 \rangle \langle R_1 | e^{-\tau \hat{H}} | R_2 \rangle \ldots \langle R_{M-1} | e^{-\tau \hat{H}} | R' \rangle$$

Analogy to groundstate QMC:

$$\Psi_0(R) = (e^{-\tau \hat{H}})^M | \Psi_T \rangle = \int dR_1 \ldots \int dR_{M-1} \langle R | e^{-\tau \hat{H}} | R_1 \rangle \langle R_1 | e^{-\tau \hat{H}} | R_2 \rangle \ldots \langle R_{M-1} | e^{-\tau \hat{H}} | \Psi_T \rangle$$

D. Ceperley, *Rev. Mod. Phys*. **67** (1995) 279.
B. Militzer, PhD thesis, see http://militzer.gl.ciw.edu

# Path Integrals in Imaginary Time

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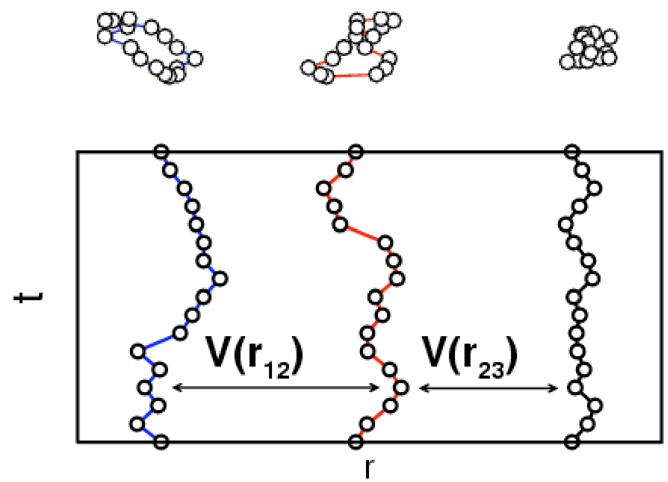
Trotter break-up:

$$\langle R|\hat{\rho}|R'\rangle = \langle R|(e^{-\tau \hat{H}})^{M}|R'\rangle = \int dR_1 \ldots \int dR_{M-1} \langle R|e^{-\tau \hat{H}}|R_1\rangle \langle R_1|e^{-\tau \hat{H}}|R_2\rangle \ldots \langle R_{M-1}|e^{-\tau \hat{H}}|R'\rangle$$

Path integral and action:



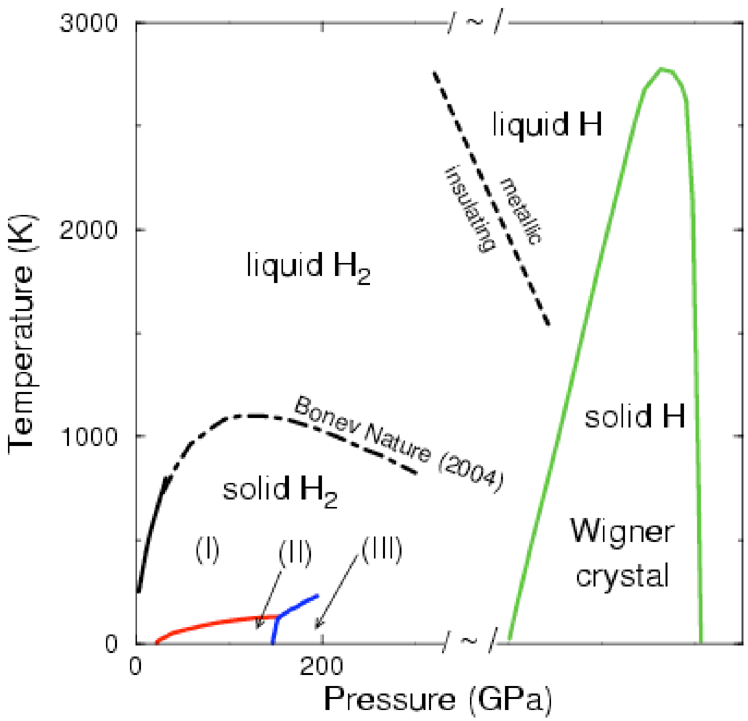

$$\langle R|\hat{\rho}|R'\rangle = \oint_{R \to R'} dR_t \, e^{-S[R_t]}$$

$$S[R_t] = \sum_{i=1}^{M} \frac{(R_{i+1} - R_i)^2}{4\lambda\tau} + \frac{1}{2}[V(R_i) + V(R_{i+1})]$$

Start with solution of 2-particle problem ⇒ improved pair action

# Example for PIMC with distinguishable particles: Melting of Atomic Hydrogen

**At extremely high pressure, atomic hydrogen is predicted to form a Wigner crystal of protons (b.c.c. phase)**




Electron gas is highly degenerate. Model calculation for a one-component plasma of protons.

Coulomb simulations have been preformed by Jones and Ceperley, Phys. Rev. Lett. (1996).

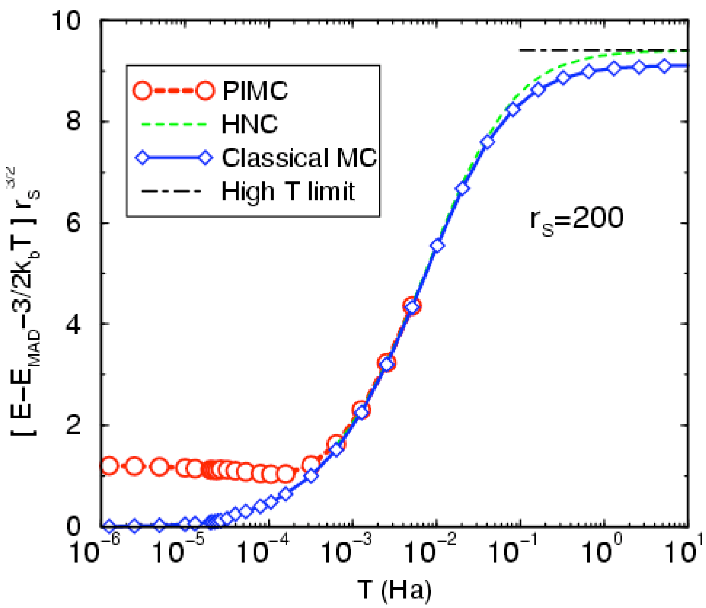
Here, we include electron screening effects by including Thomas Fermi screening leading to a Yukawa pair potential:

$$V(r) = \frac{Z^2}{r} e^{-r / D_s}$$

1) Distinguish between classical and quantum melting.
2) Can a liquid exist at T=0 in between the molcular and atomic solid? Superfluidity and superconductivity in liquid hydrogen? (Babaev & Ashcroft)

# Simulation of Hydrogen Melting

## Wigner crystal of protons studied with PIMC




**Compare classical Monte Carlo with PIMC results:**

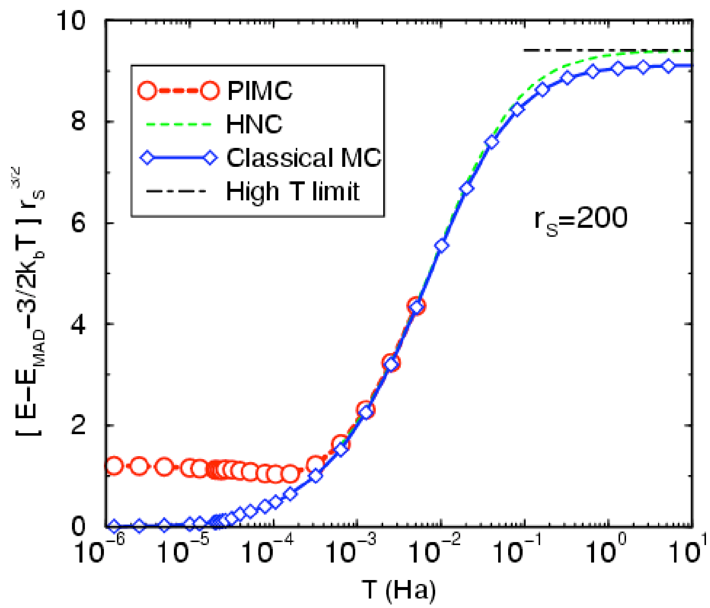
1) **At high T, all particles behave classically, if the thermal de Broglie length is small:**

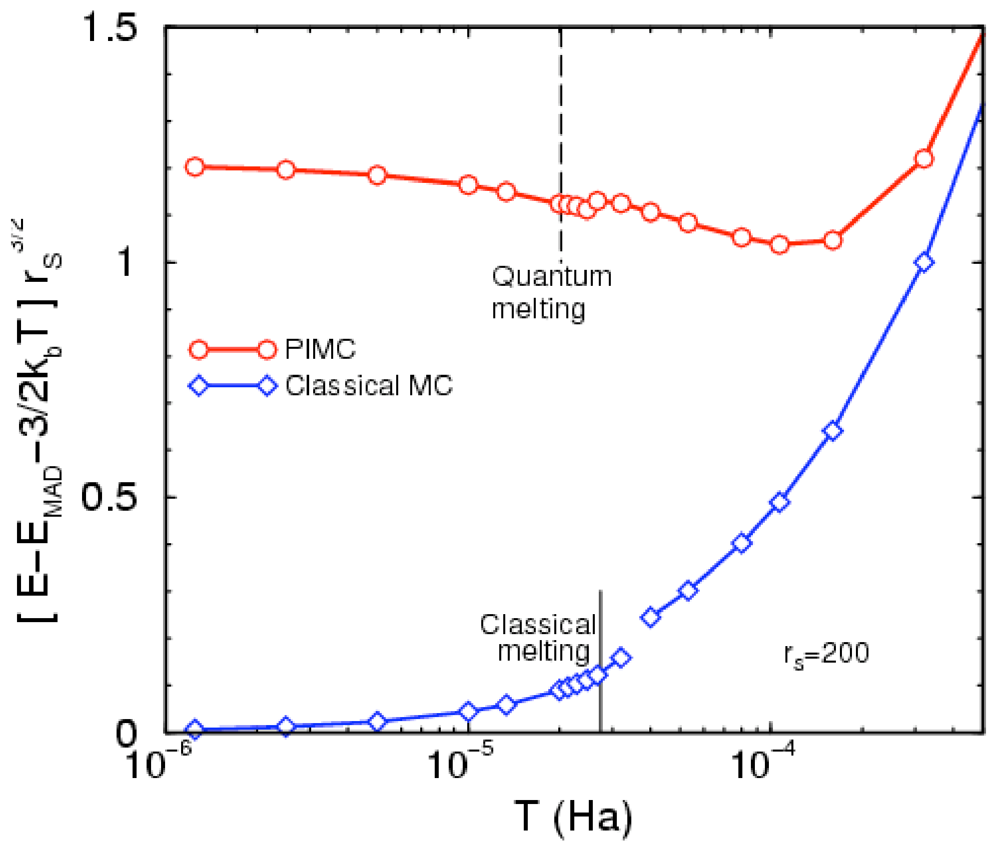
$$r_S >> \lambda_d \quad , \quad \lambda_d = \sqrt{\frac{h^2}{2\pi\, m\, k_b T}}$$

2) **At low T, quantum simulations show a much higher energy due to the zero point motion.**

# Simulation of Hydrogen Melting

## Wigner crystal of protons studied with PIMC

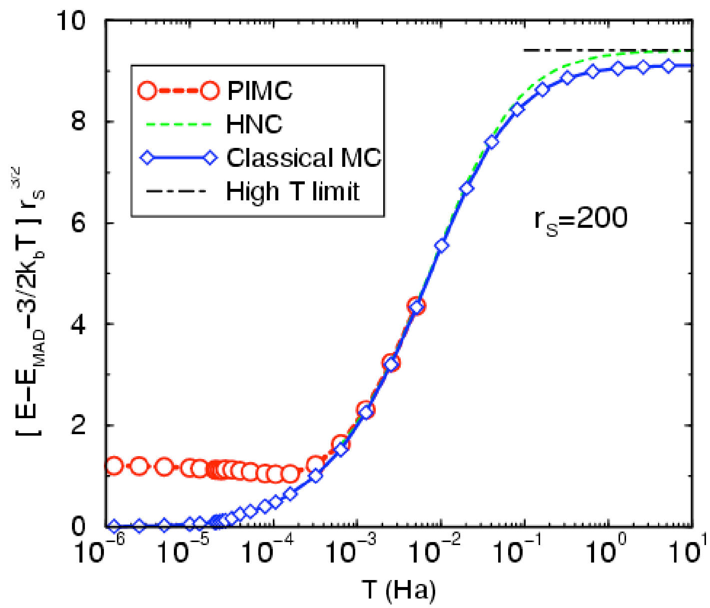


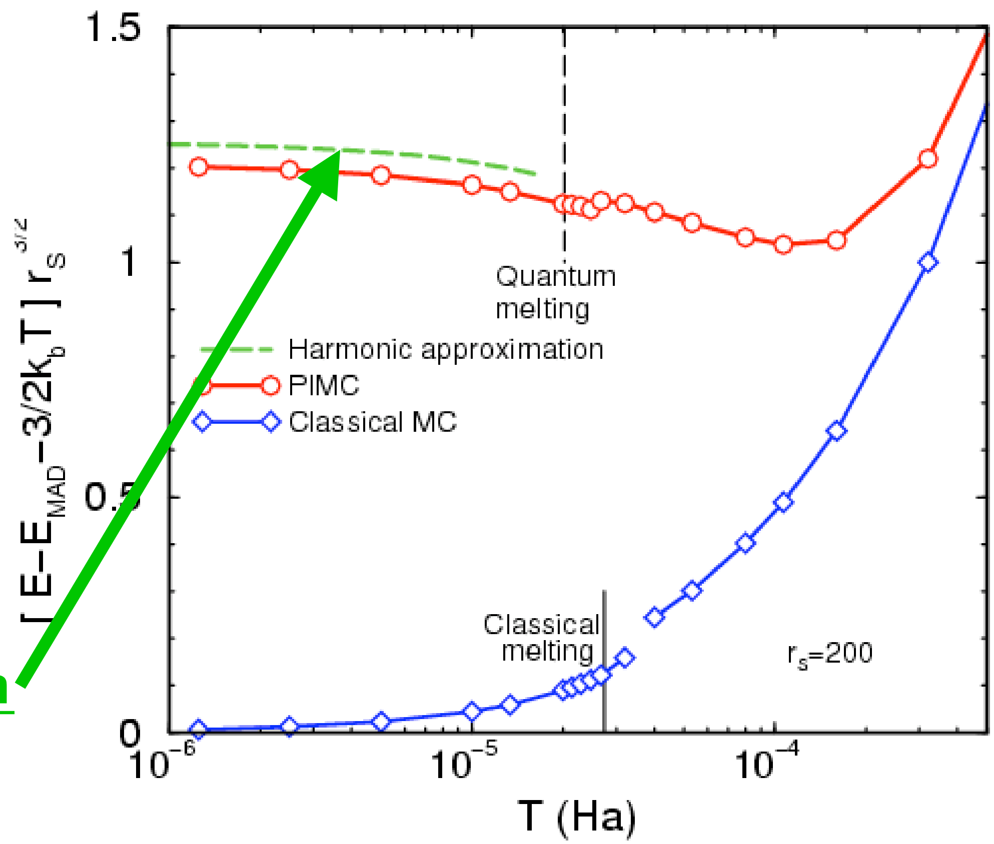




1) **PIMC leads to an exact solution of the Schroedinger equation at any T (for distinguishable particles)**
2) **Thermal lattice vibrations are treated exactly (PIMC can only study equilibrium properties, no dynamics)**

# Simulation of Hydrogen Melting

## Comparison with harmonic lattice approximation



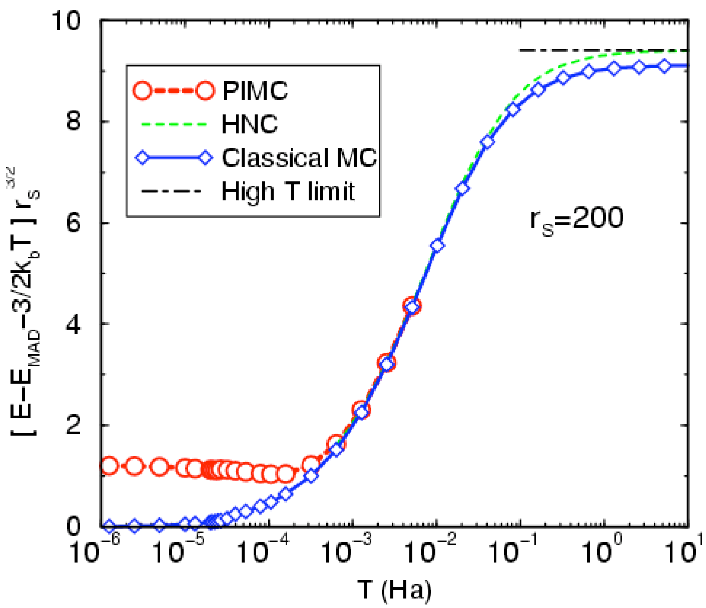

**Harmonic lattice approximation**

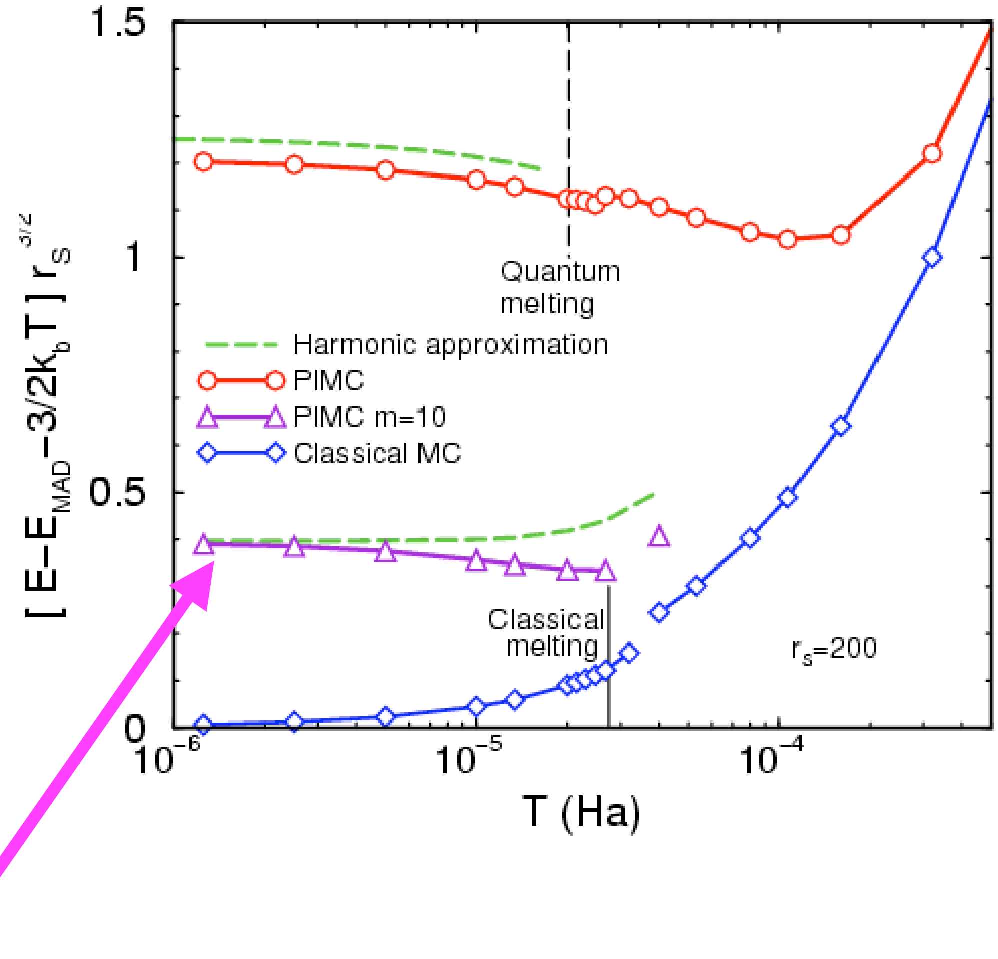
$$D_{ij} = \frac{1}{\sqrt{m_i m_j}} \frac{\partial^2 V}{\partial R_i \partial R_j} \quad , \quad \left| D - 1\omega^2 \right| = 0$$

**In the HLA, the protons are too localized because they are light particle, probe the anharmonic regions of the potential.**

# Simulation of Hydrogen Melting

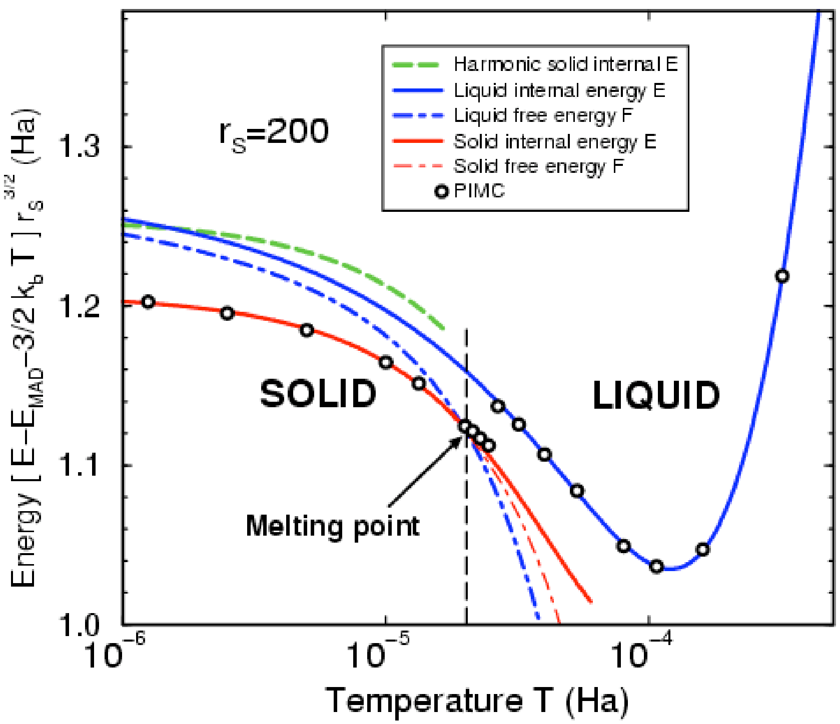
## Wigner crystal of protons studied with PIMC

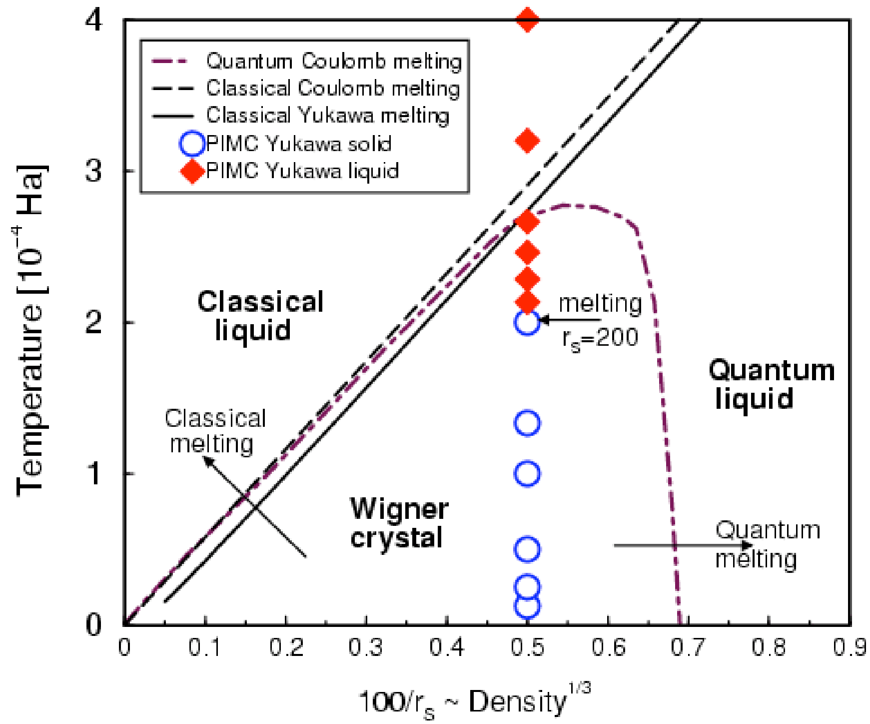



**For heavier particles, the HLA works much better.**

# Free energy calculations predict that melting temperature is reduced by quantum effects




**Free energies by thermodynamic integration of the internal energy**

$$\beta_1 F(\beta_1) - \beta_0 F(\beta_0) = \int_{\beta_0}^{\beta_1} E(\beta)\, d\beta$$

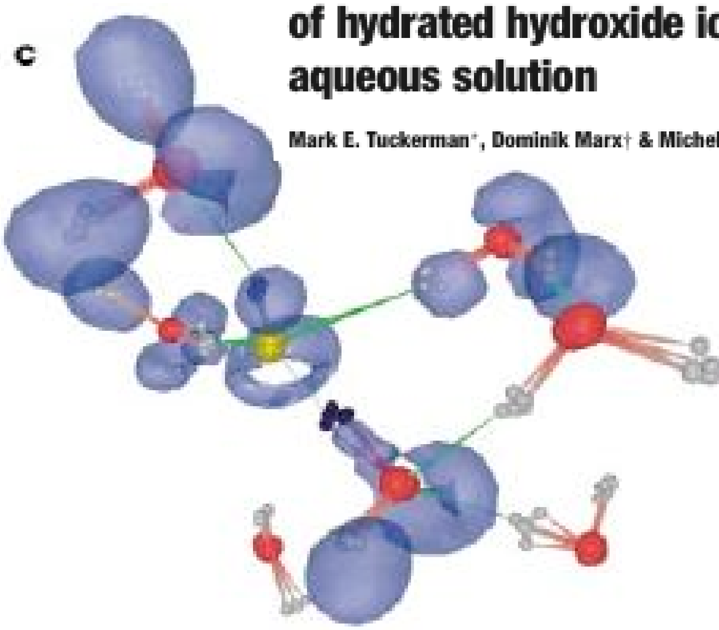
**Quantum motion of hydrogen nuclei reduces the melting temperature.**

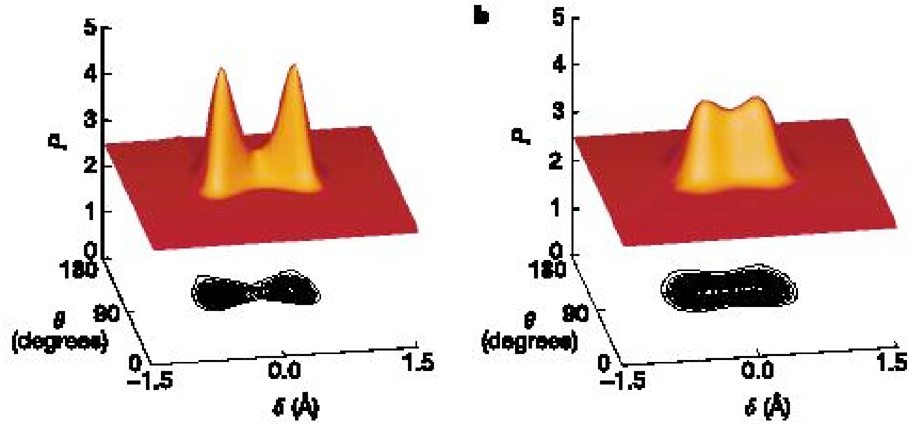
Militzer, Graham, Journal of Physics and Chemistry of Solids, in press (2006), also see cond-mat.

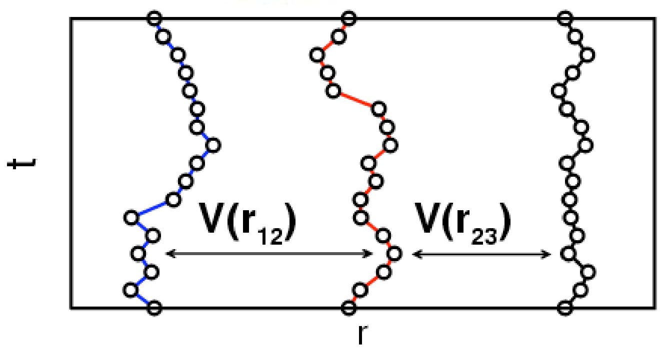
# PIMC for the nuclei based on forces derived with DFT (how to make water softer)

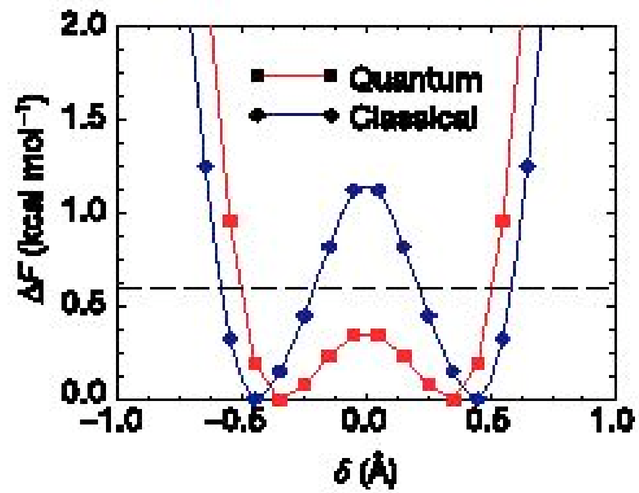
**The nature and transport mechanism of hydrated hydroxide ions in aqueous solution**

Mark E. Tuckerman*, Dominik Marx† & Michele Parrinello‡§



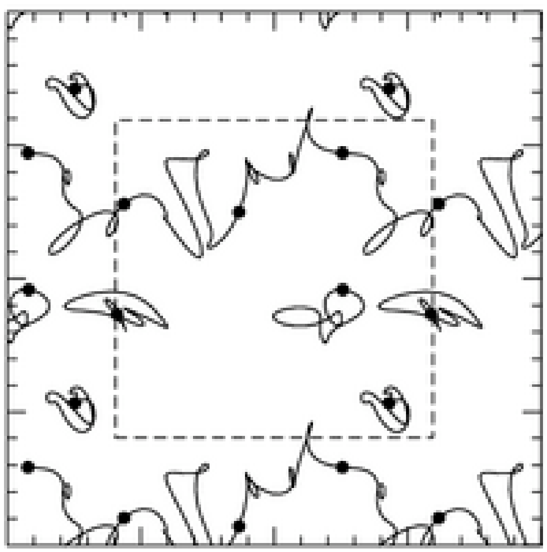
# Particle Statistics

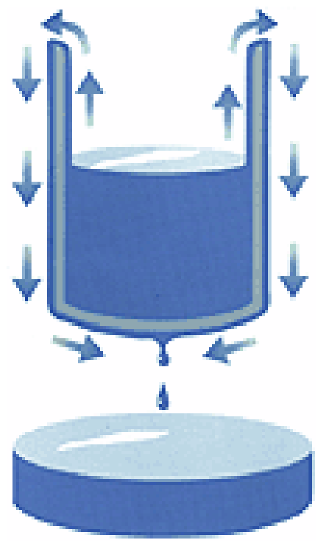
## leads to exchange effects represented by permutations.

Symmetry leads to bosonic and fermionic path integrals

$$\langle R \,|\, \hat{\rho}_{F/B} \,|\, R \rangle = \sum_{P} (\pm 1)^{P} \int dR_1 \ldots \int dR_{M-1} \langle R \,|\, e^{-\tau \hat{H}} \,|\, R_1 \rangle \ldots \langle R_{M-1} \,|\, e^{-\tau \hat{H}} \,|\, PR \rangle$$

Bosons: Long permutation cycles, only positive contributions ⇒ superfluidity in $^4$He





The superfluid fraction, $\rho_S$, can be derived from the winding number, $\mathcal{W}$, in PIMC simulations,

$$\frac{\rho_S}{\rho} = \frac{\langle W^2 \rangle}{2\lambda\beta N}$$

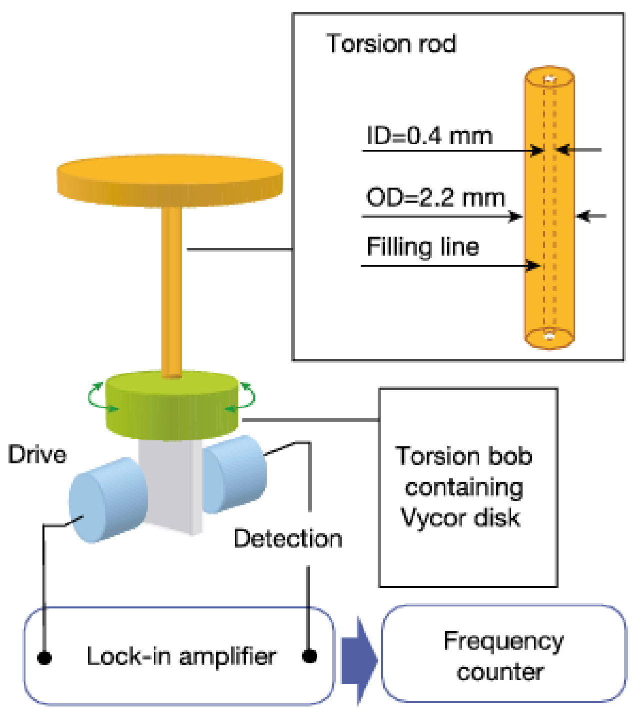
D. Ceperley, *Rev. Mod. Phys*. **67** (1995) 279.

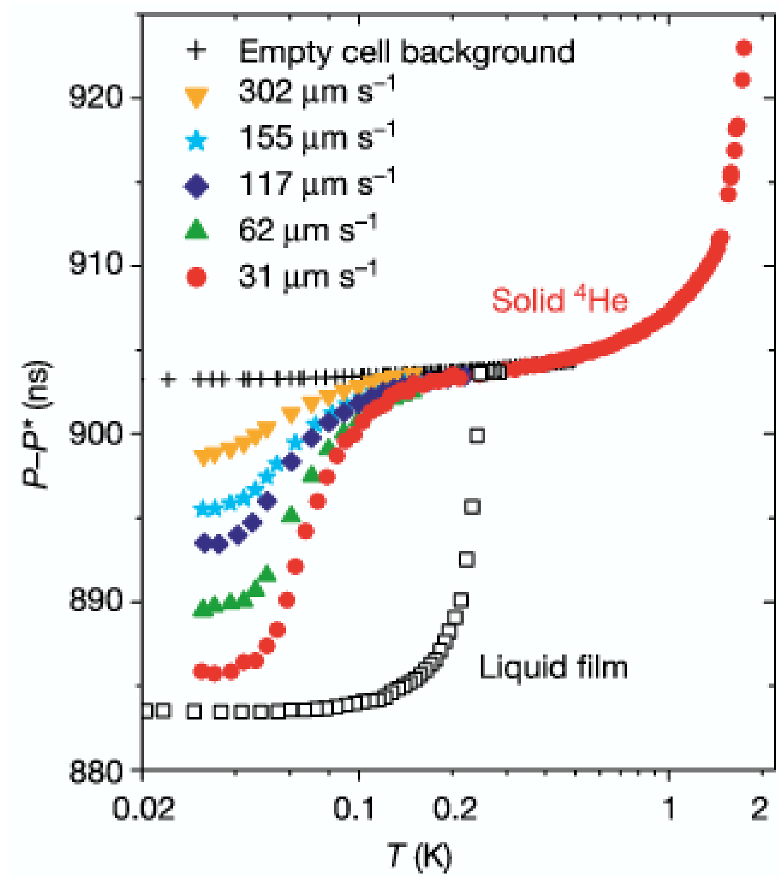
## Kim & Chan [Nature 427 (2004) 225] demonstrate that solid bulk $^4$He at 62 bar exhibits superfluidity.

**Probable observation of a supersolid helium phase**

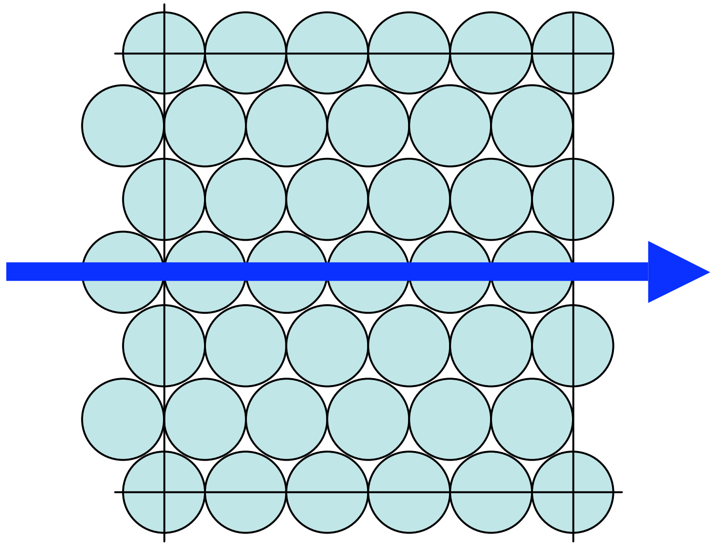
**E. Kim & M. H. W. Chan**

*Department of Physics, The Pennsylvania State University, University Park, Pennsylvania 16802, USA*

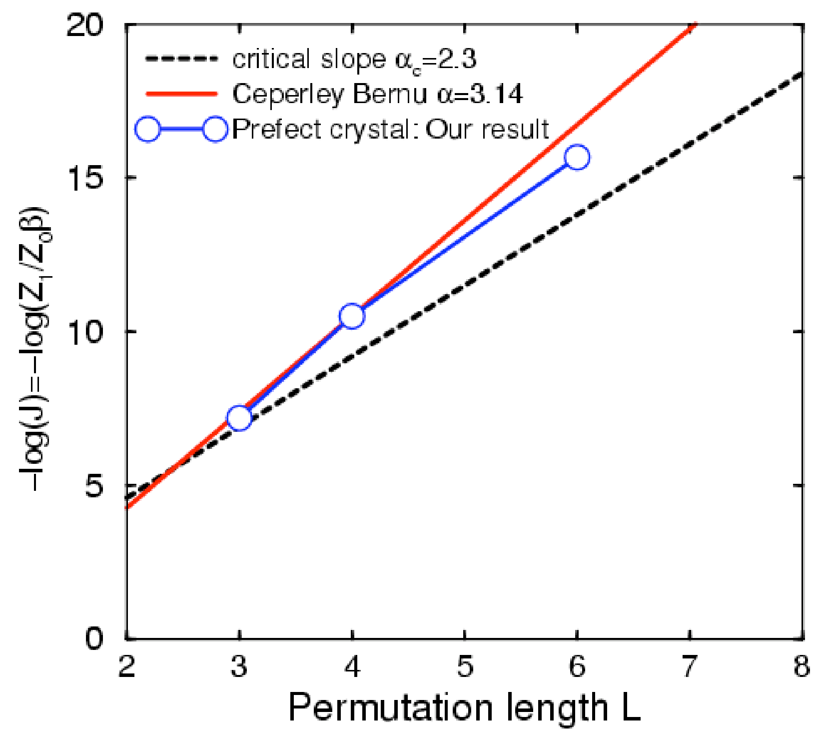


# Ceperley-Bernu approach: Exchange frequency calculation in perfect crystal



$$\frac{Z_P}{Z_0} = \frac{\int dR \langle R | (e^{-\tau\hat{H}})^M | PR \rangle}{\int dR \langle R | (e^{-\tau\hat{H}})^M | R \rangle} \equiv J_P \square$$




- For a **fixed** permutation, the free energy cost, *J*, is calculated using a switching method (Bennett).
- Kikuchi model: The slope of *J(L)* must be less then **2.3** to support superfluidity.
- Ceperley & Bernu (PRL 2004) showed that a perfect crystal cannot become superfluid.

# Particle Statistics

## leads to exchange effects represented by permutations.

Symmetry leads to bosonic and fermionic path integrals

$$\langle R|\rho_{F/B}|R'\rangle = \sum_{P} (\pm 1)^{P} \int dR_1 \ldots \int dR_{M-1} \langle R|e^{-\tau\hat{H}}|R_1\rangle \ldots \langle R_{M-1}|e^{-\tau\hat{H}}|PR'\rangle$$

<u>Fermions:</u> Cancellation of positive and negative contributions

$\Rightarrow$ Fermion sign problem,

efficiency $e^{-\beta\Delta}$

<u>Fixed node approximation</u>

$$\langle R|\rho_{F}|R'\rangle = \sum_{P} (-1)^{P} \oint_{\rho_T \geq 0} dR_t\, e^{-S[R_t]}$$

# Comparison: T=0 and T>0 Fermion Methods

Analogy to Ground State Methods

| T = 0 | T > 0 |
|---|---|
| $\Psi_{GS}(\mathbf{R})$ | $\rho(\mathbf{R},\mathbf{R}';\beta) = \Sigma_s e^{-\beta E_s}\Psi_s(\mathbf{R})\mathbf{\Psi_s}(\mathbf{R}')$ |
| $E \leq <\Psi\|H\|\Psi> / <\Psi\|\Psi>$ | $F \leq \mathrm{Tr}[\tilde{\rho}H] + kT\ \mathrm{Tr}[\tilde{\rho}\ln\tilde{\rho}] \quad \tilde{\rho} = \rho/\mathrm{Tr}[\rho]$ |

1. Effective Single Particle Level

$$\Psi_{KS}(\mathbf{R}) = \begin{vmatrix} \Phi_1(r_1) & \dots & \Phi_N(r_1) \\ \dots & \dots & \dots \\ \Phi_1(r_N) & \dots & \Phi_N(r_N) \end{vmatrix}$$

$$\rho(\mathbf{R},\mathbf{R}';\beta) = \begin{vmatrix} \rho^{[1]}(r_1,r_1';\beta) & \dots & \rho^{[1]}(r_N,r_1';\beta) \\ \dots & \dots & \dots \\ \rho^{[1]}(r_1,r_N';\beta) & \dots & \rho^{[1]}(r_N,r_N';\beta) \end{vmatrix}$$

LDA: $\epsilon_s\Phi_s = -\frac{\nabla^2}{2}\Phi_s + V_{eff}\Phi_s$

Variational solution of many-body Bloch Equation

2. Correlations beyond LDA or Mean Field

| T = 0 | T > 0 |
|---|---|
| Jastrow | Finite Temperature Jastrow |
| $\Psi_{GS}(\mathbf{R}) = \Psi_{KS}(\mathbf{R})\,\Pi_{i,j}\,f(r_{ij})$ | $\rho(\mathbf{R},\mathbf{R}';\beta) = \rho_{MF}(\mathbf{R},\mathbf{R}';\beta)\,\Pi_{i,j}\,f(r_{ij},r_{ij}';\beta)$ |

3. Diffusion QMC | Restricted PIMC

# Derivation of a Variational Density Matrix

**(see Militzer, Pollock, Phys. Rev. E 61 (2000) 3470)**

Bloch equation: $$-\frac{\partial \rho}{\partial \beta} = \mathcal{H}\rho$$

Ansatz for density matrix

$$\rho(\mathcal{R},\mathcal{R}';\beta) = \rho(\mathcal{R}, q_1, \ldots, q_m) \qquad q_k = q_k(\mathcal{R}',\beta)$$

Variational principle: $\delta I = 0$

$$I\left(\frac{\partial \rho}{\partial \beta}\right) = \int d\beta \int d\mathcal{R} \left(\frac{\partial \rho}{\partial \beta} + \mathcal{H}\rho\right)^2$$

$\Rightarrow$ ordinary differential equations for $q_k$ in imaginary time

Slater determinant: $\rho(\mathcal{R},\mathcal{R}';\beta) = \left\|\rho^{[1]}(\mathbf{r}_i,\mathbf{r}'_j;\beta)\right\|_{ij}$

Gaussian Ansatz:

$$\rho^{[1]}(\mathbf{r},\mathbf{r}',\beta) = (\pi w)^{-3/2} \exp\left\{-\frac{1}{w}(\mathbf{r}-\mathbf{m})^2 + d\right\}$$

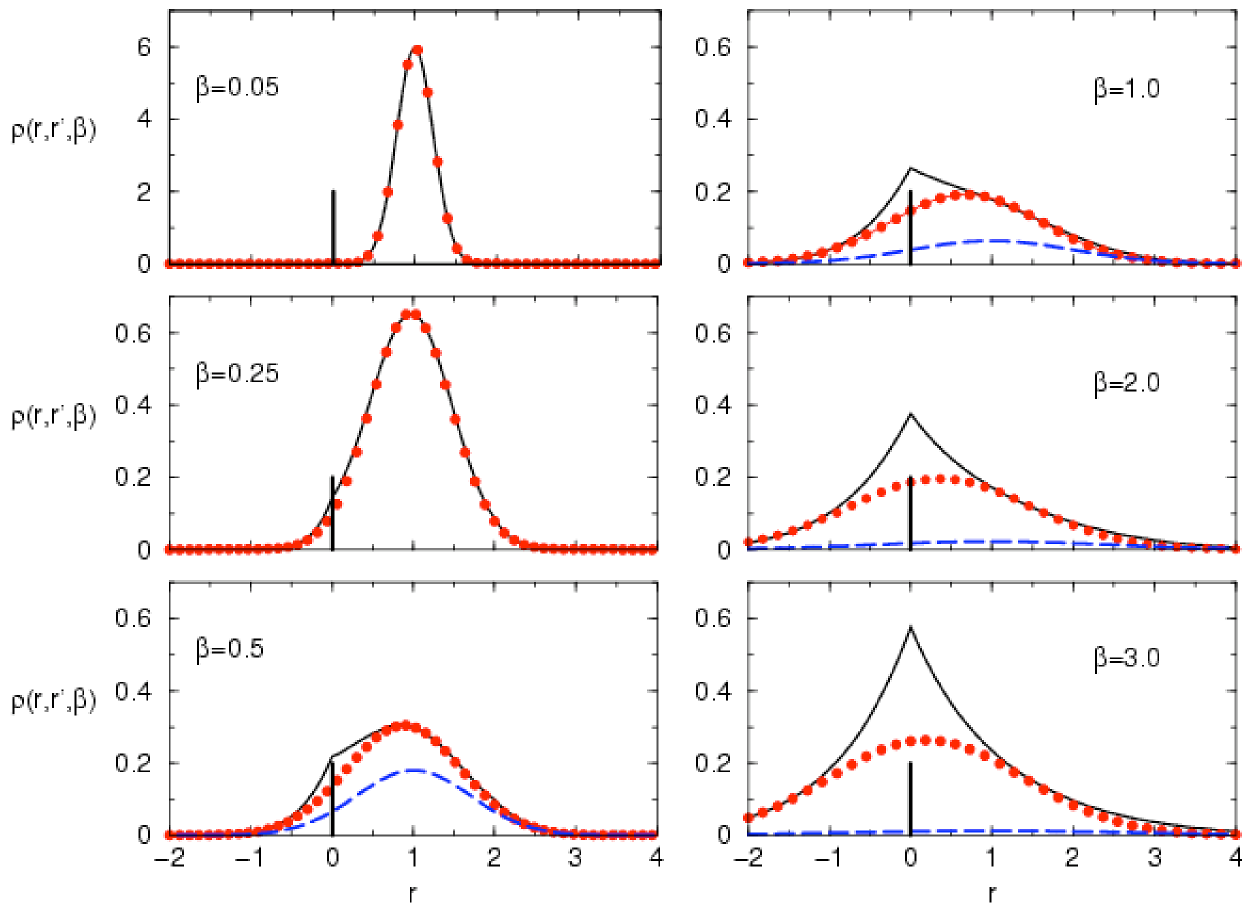
Variational parameters: $\mathbf{m}$ ... mean position $(= r')$
$w$ ... squared width $(=4\lambda\beta)$
$d$ ... amplitude $(=0)$

# Derivation of a Variational Density Matrix

**(see Militzer, Pollock, Phys. Rev. E 61 (2000) 3470)**

Gaussian Ansatz:

$$\rho^{[1]}(\mathbf{r},\mathbf{r}',\beta) = (\pi w)^{-3/2} \exp\left\{-\frac{1}{w}(\mathbf{r}-\mathbf{m})^2 + d\right\}$$



# Why are there no PIMC calculations for elements heavier than helium yet?

Problem 1: Nonlocal pseudopotentials in fermionic path integrals

$$\langle R \mid \hat{\rho}_{n.l.} \mid R' \rangle = \langle R \mid e^{-\beta[\hat{T}+\hat{V}_{n.l.}]} \mid R' \rangle$$

$\Rightarrow$ Sign problem even for the 1-particle scattering problem.

Problem 2: More accurate nodes at low T.

Make a step forward by making one step back first:

Reintroduce Born-Oppenheimer approximation:

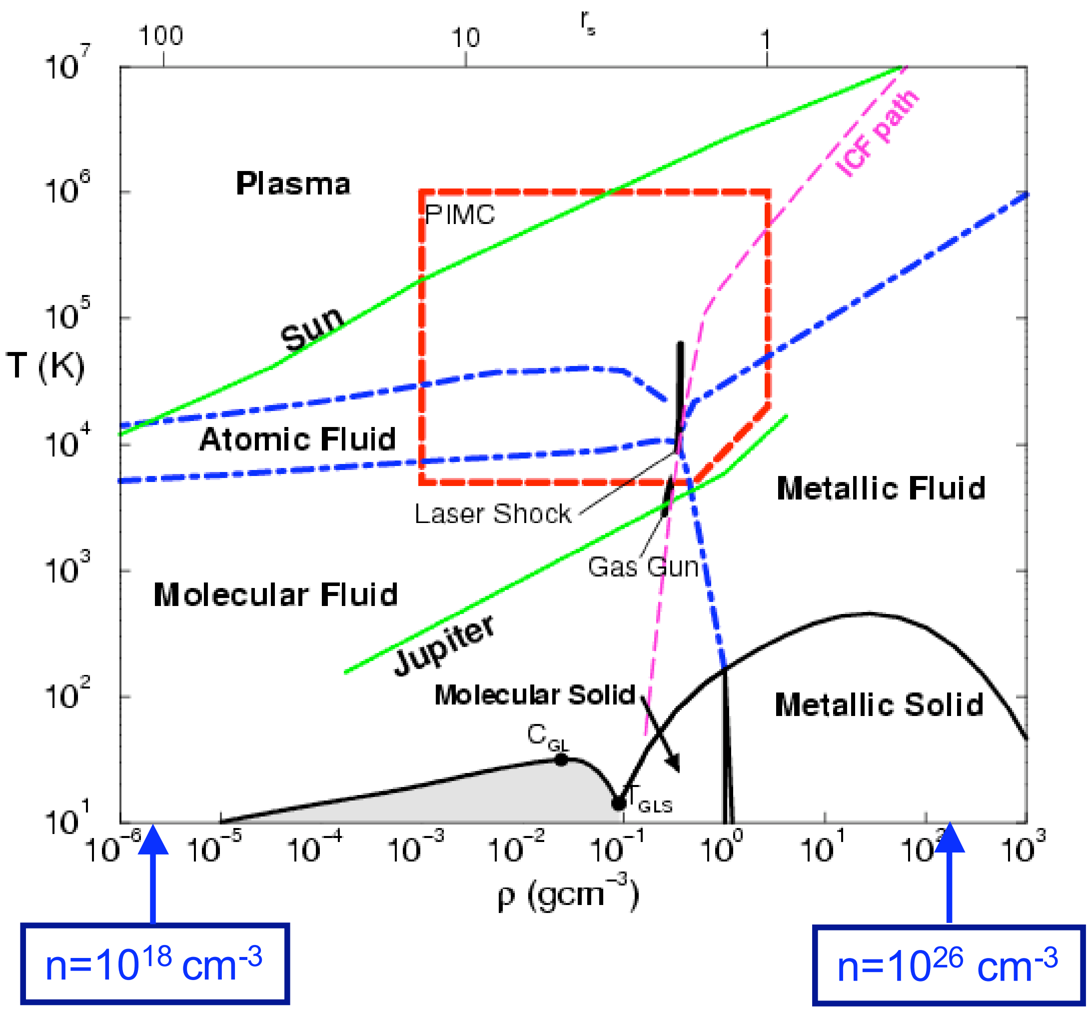
Classical MC for the ions ($T_{ion} > 0$)

QMC for the electrons ($T_{el} = 0$)

(Delaney, Pierleonie, Ceperley)

# High Temperature Hydrogen Phase Diagram

## Temperature vs. density

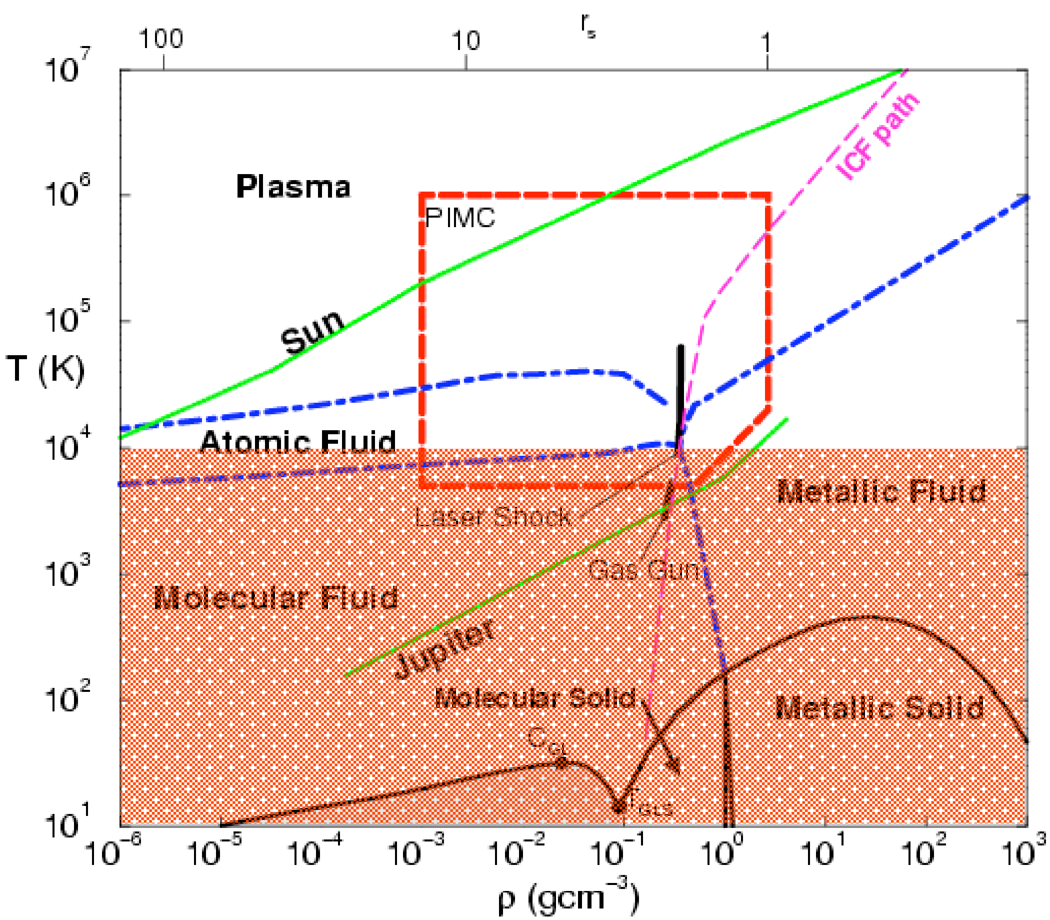


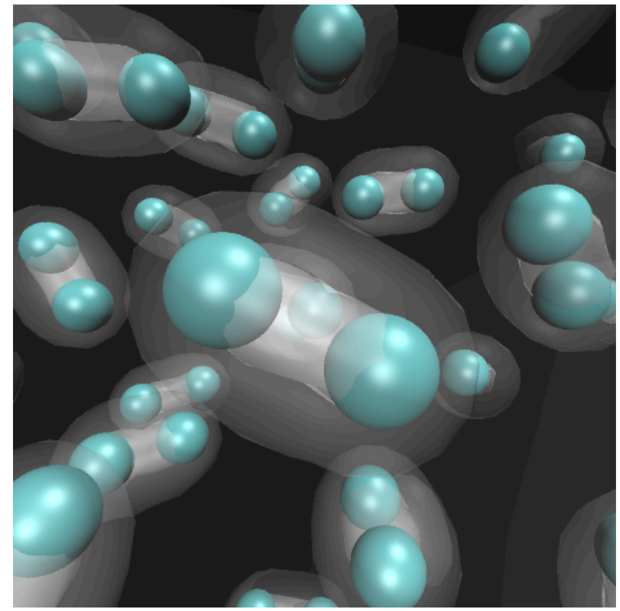

EOS relevant for:

- Jovian planets, sun
- Inertial confinement fusion (ICF)
- Pulse powered plasmas

PIMC applicable at: T>5000K

# 1) Path integral Monte Carlo for T>5000K
# 2) Density functional molecular dynamics below



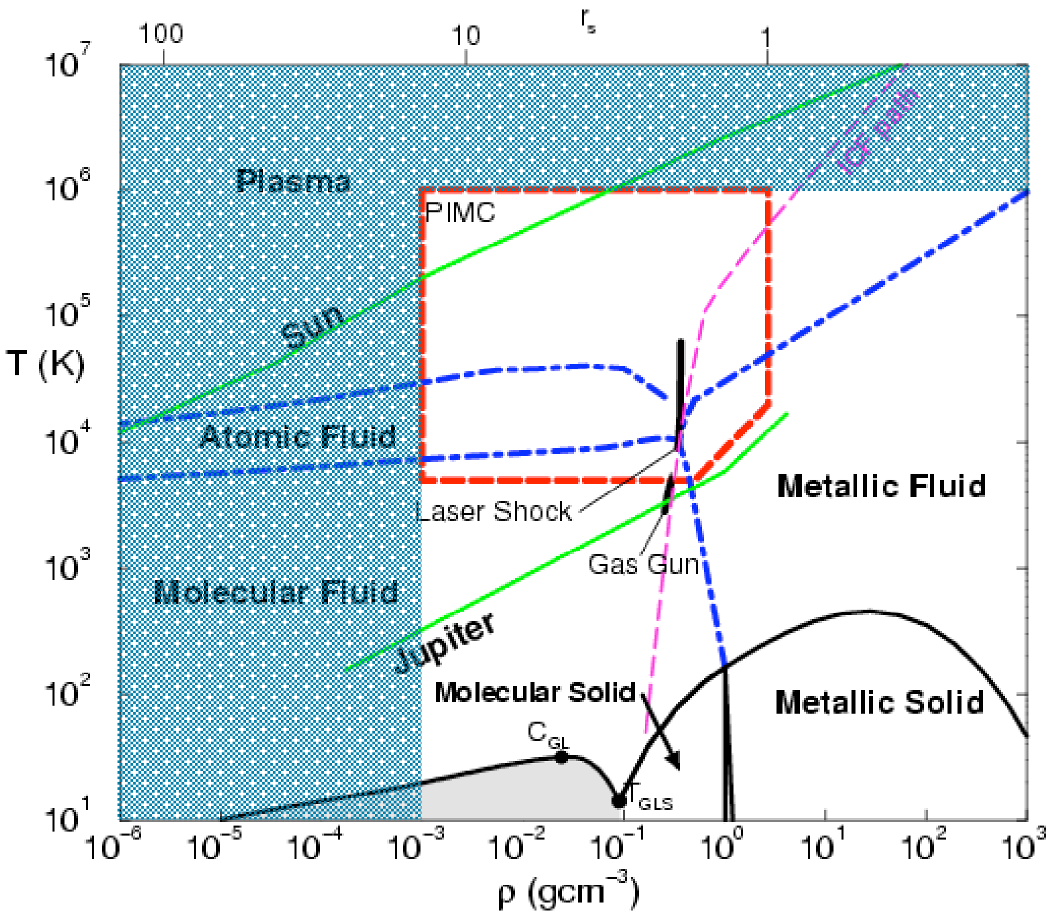



Born-Oppenheimer approx.
MD with classical nuclei:

**F = m a**

Forces derived DFT with electrons in the instantaneous ground state.

# Use analytical (chemical) models at low density and very high temperature




Free energy model to describe weakly interacting chemical species:

$H_2$, H, $H^+$, $e^-$

He, $He^+$, $He^{++}$, $e^-$

Free energy is constructed but it contains free parameters to describe the interaction.

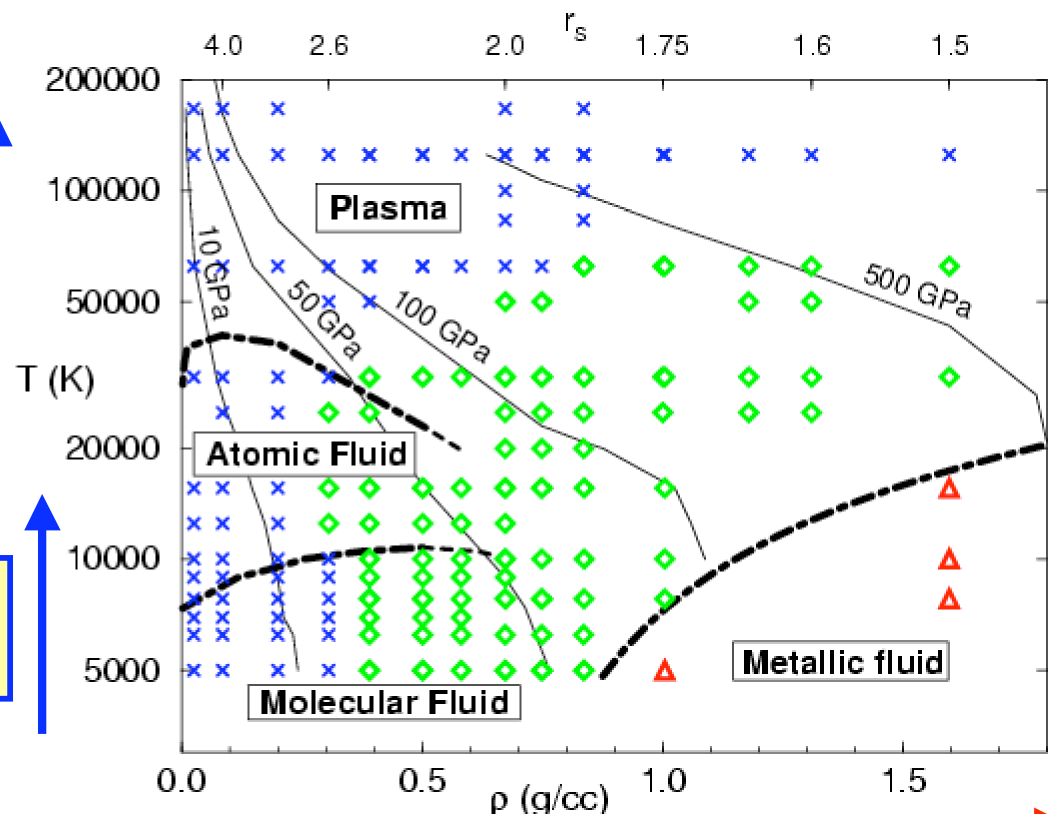
- Saumon and Chabrier
- Sesame database
- Ross model

# Deuterium Phase Diagram

## as predicted by PIMC simulations

Thermal ionization

Thermal dissociation

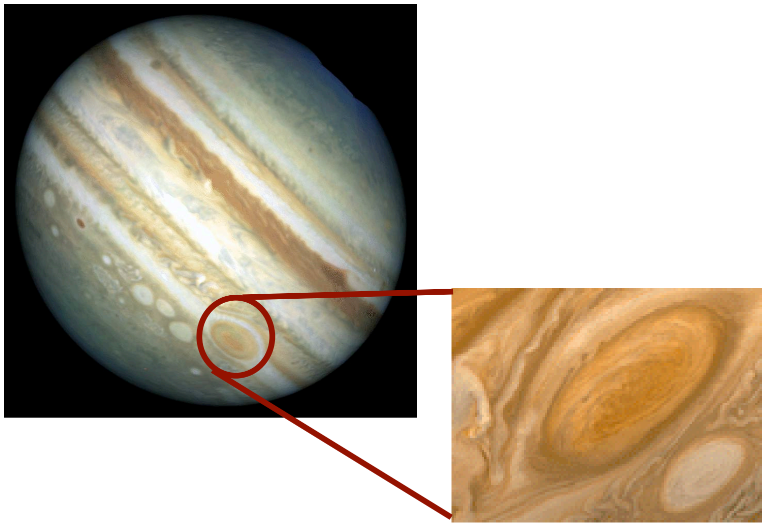


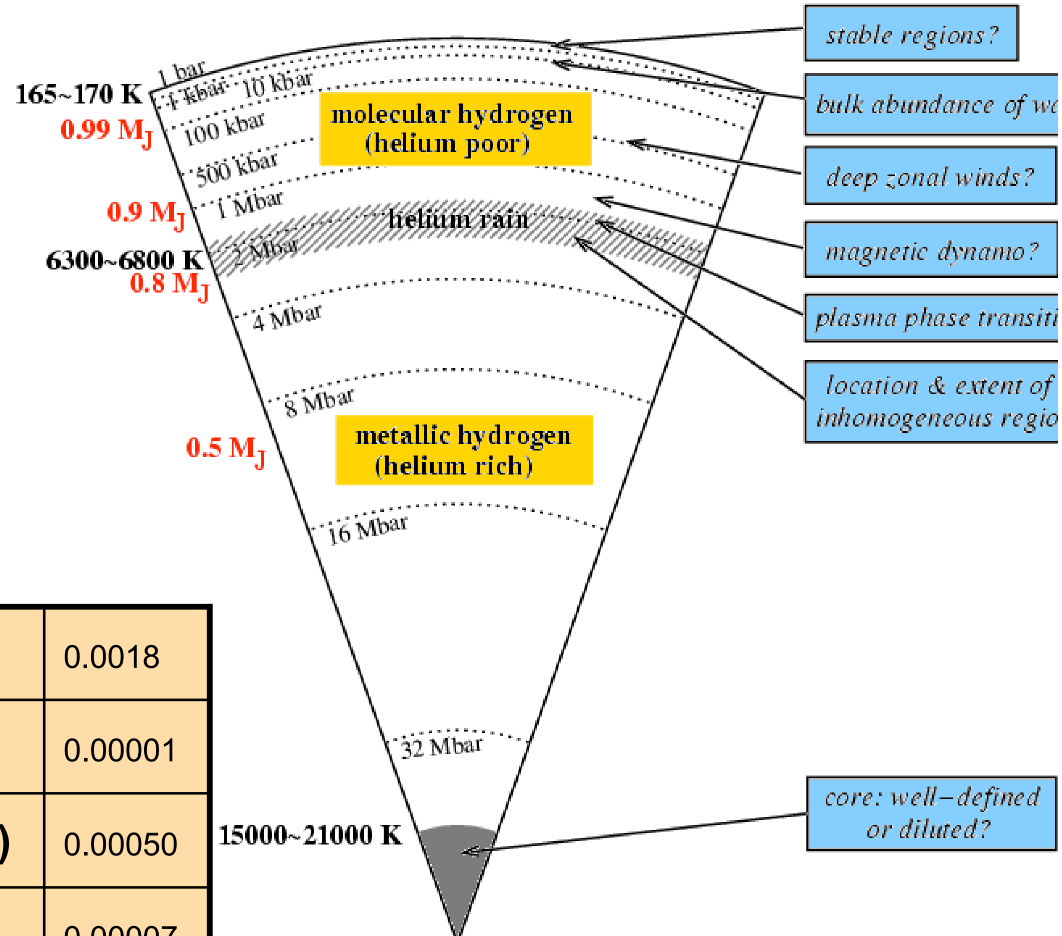

Continuous lowering of the electron degeneracy, no bound states

Entropy dissociation

Pressure dissociation

# Jupiter is well characterized only on the surface.





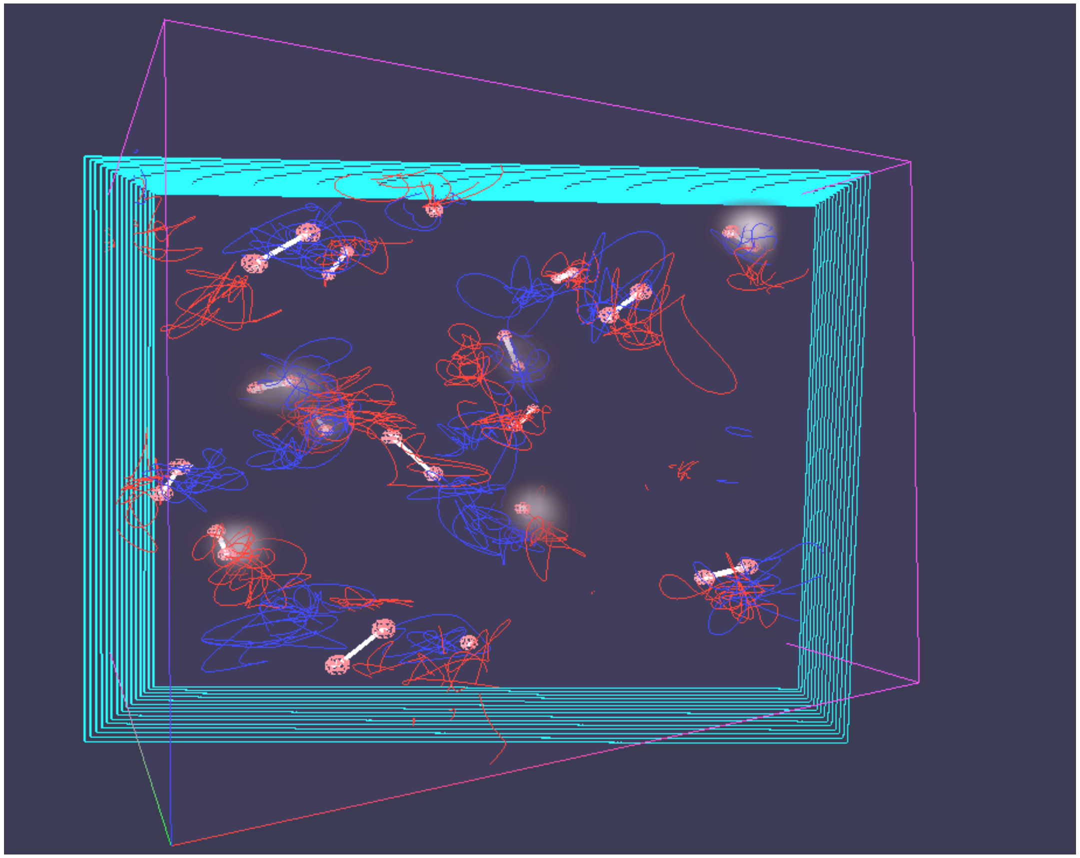

**Composition on the surface** (solar):

| | | | | | |
|---|---|---|---|---|---|
| **H** | **0.742** | 0.736 | **Ne** | **< 0.0002** | 0.0018 |
| **He** | **0.231(4)** | 0.249 | **P** | **< 0.00007** | 0.00001 |
| **C** | **0.009(2)** | 0.0029 | **S** | **0.00091(6)** | 0.00050 |
| **N** | **< 0.012** | 0.00085 | **Ar** | **< 0.00015** | 0.00007 |
| **O** | **< 0.0035** | 0.0057 | **"Z"** | **0.027** | 0.015 |

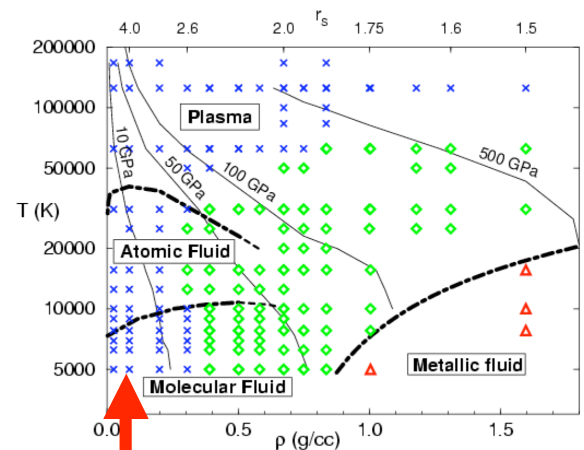
Guillot et al. (Jupiter book, 2002, chap.3 )

# Molecular Hydrogen

## Snapshot from a PIMC simulation with 32 protons and electrons



2 protons (pink spheres) and spin-up and one spin-down electron form one $H_2$ molecule.

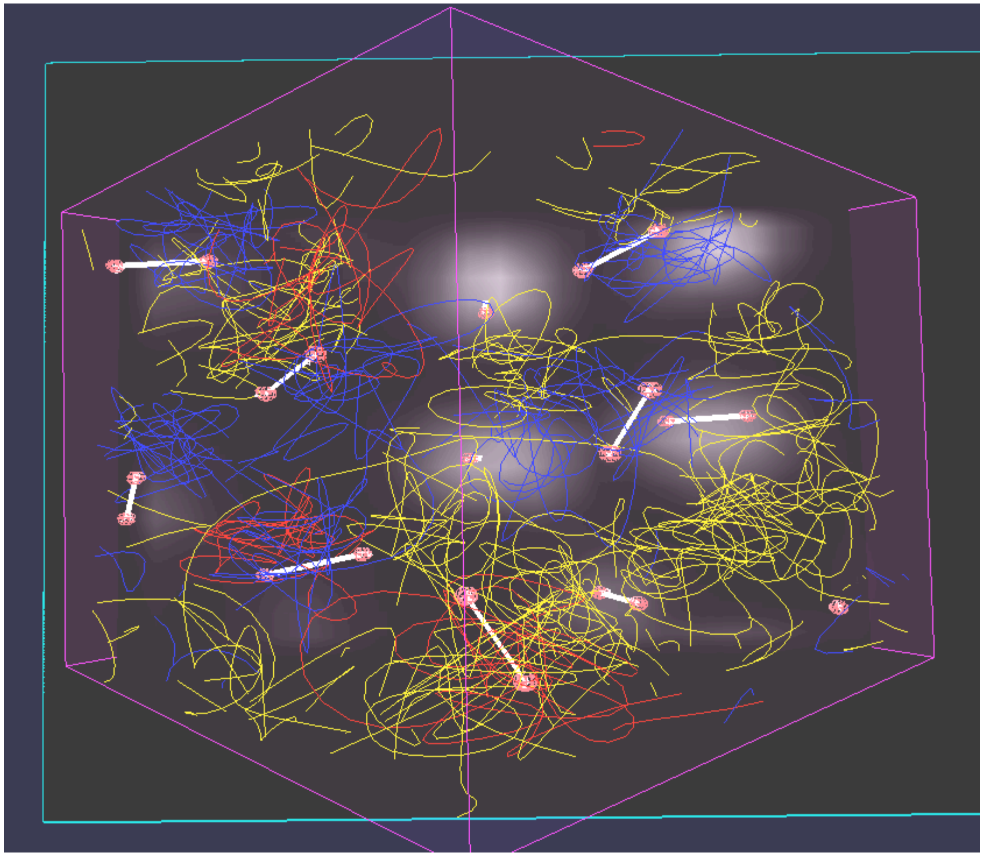



T=5000K, $r_s$=4

100% molecules, weakly interacting

# Molecular Hydrogen

## Snapshot from a PIMC simulation with 32 protons and electrons



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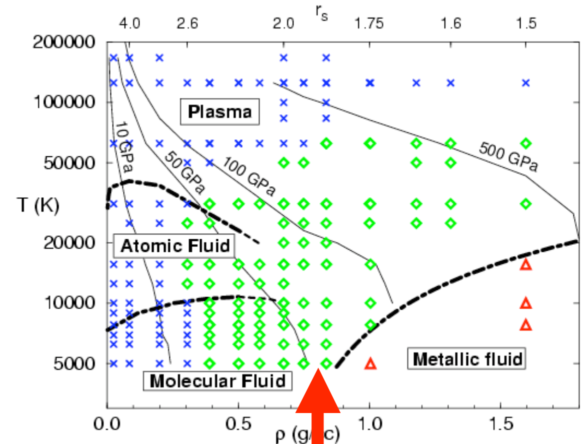
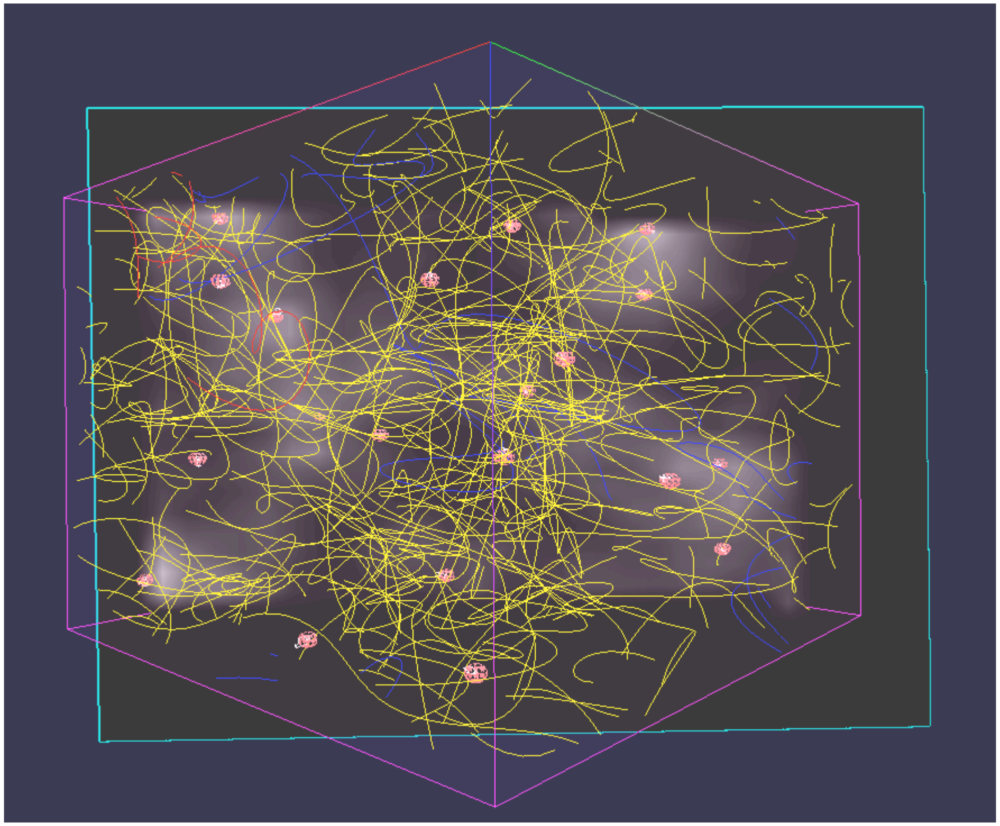



T=5000K, $r_s$=1.86

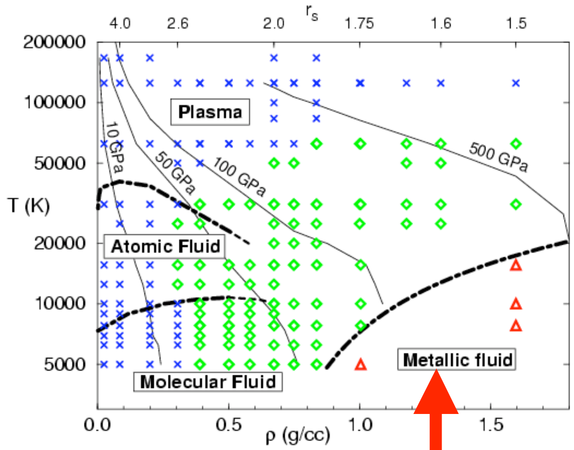
- strongly interacting molecules, close to pressure dissociation
- Electrons are degenerate, partially delocalized
- Electron paths are permuting

# Metallic Hydrogen

## Snapshot from a PIMC simulation with 32 protons and electrons



Free protons (pink spheres) and delocalized electrons.

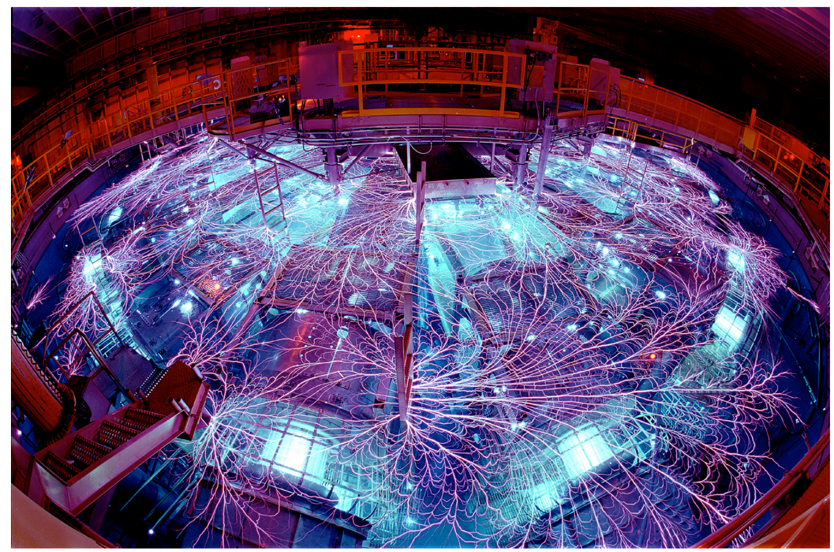



T=5000K, $r_s$=1.6

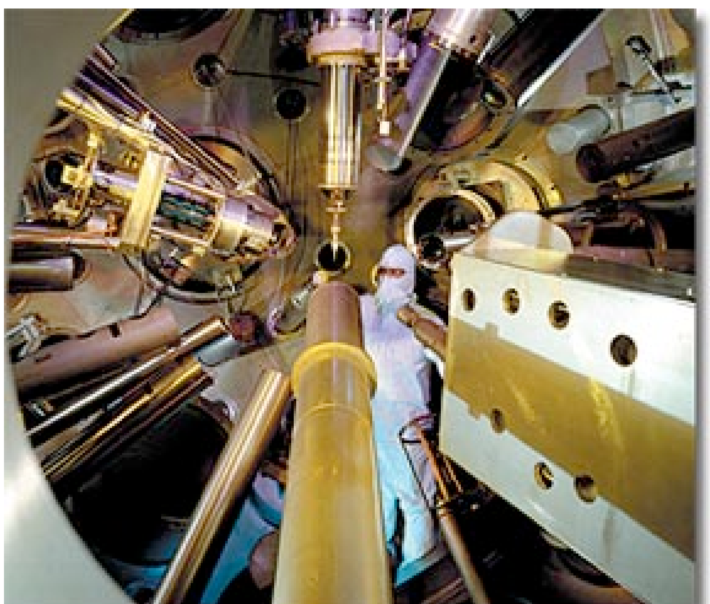
- Pressure dissociation, free protons
- Degenerate electron gas
- High number of permutations

# Study planetary interiors in the laboratory: shock wave experiments

1) Two-stage gas gun (Livermore)
20 GPa in deuterium



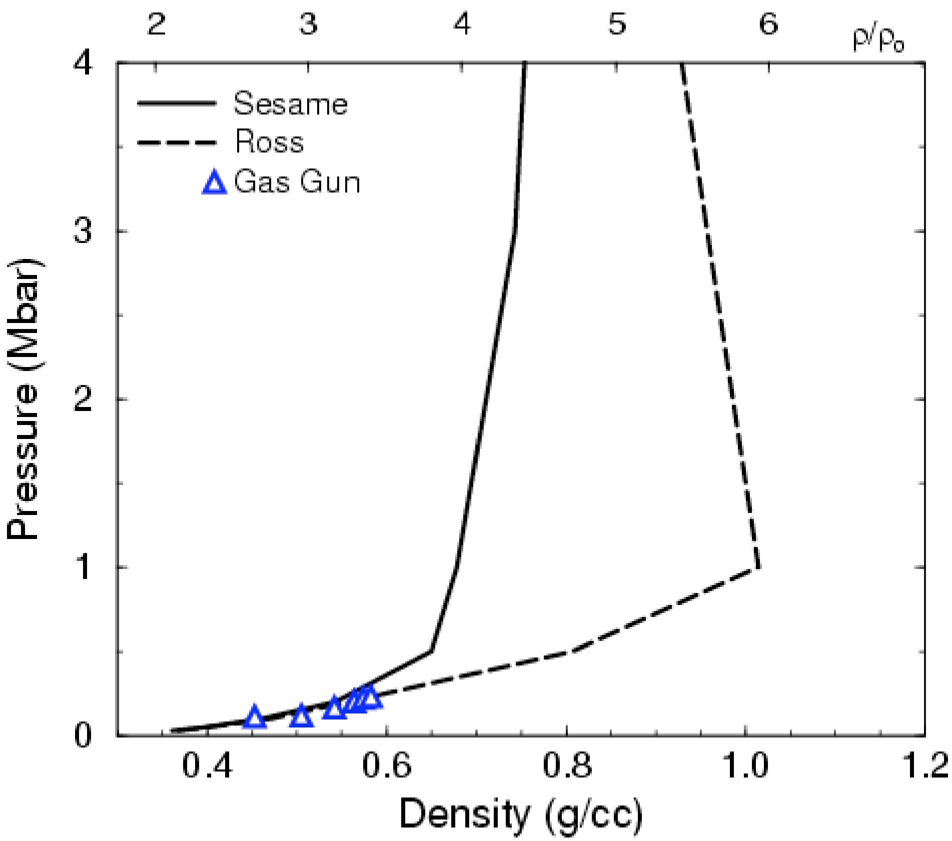
3) Z capacitor bank (Sandia) 175 GPa

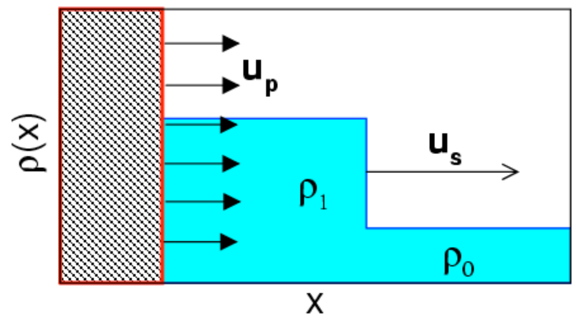


2) Nova laser (Livermore) 340 GPa

4) NIF…

# Shock wave measurements determine the EOS on the Hugoniot curve




Conservation of mass, momentum and energy yields:

$$\frac{\rho}{\rho_0} = \frac{u_s}{u_s - u_p}$$

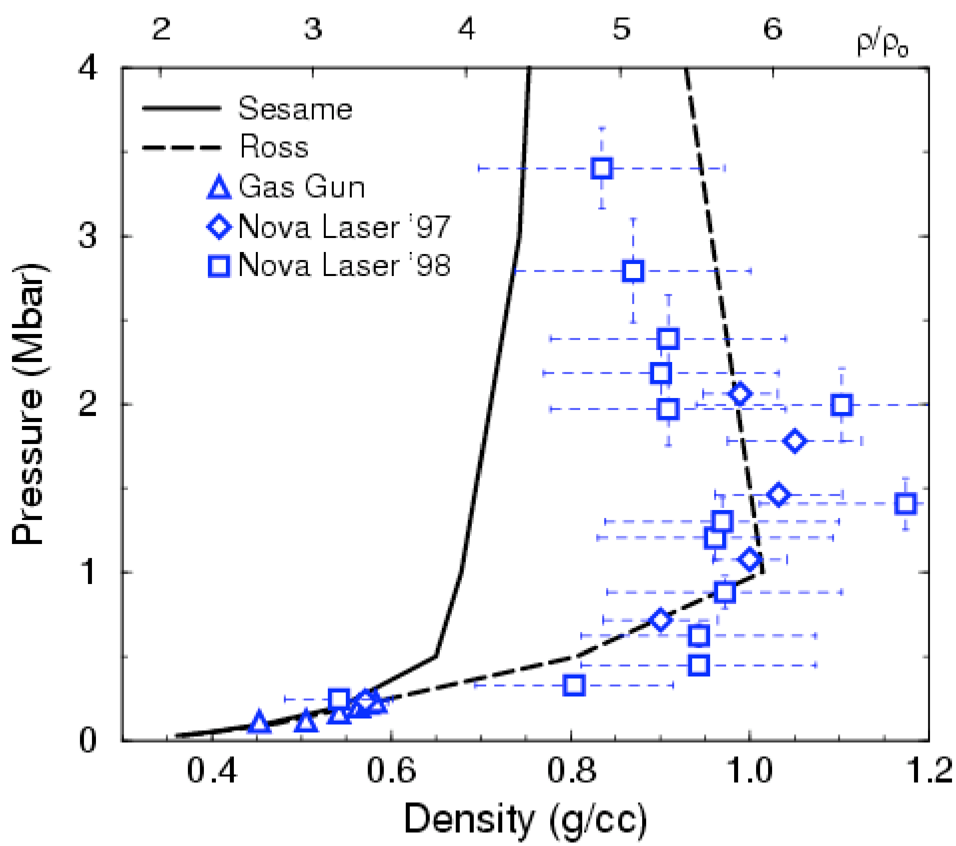
$$p - p_0 = \rho_0 u_s u_p$$

$$E - E_0 = \frac{1}{2}(V_0 - V)(P + P_0)$$

Gas gun (LLNL), Sesame model (Kerley), linear mixing model (M.Ross)

# Deuterium Hugoniot

**Nova laser shock wave experiments reached 3.4 Mbar**




Why is the compressibility so high?

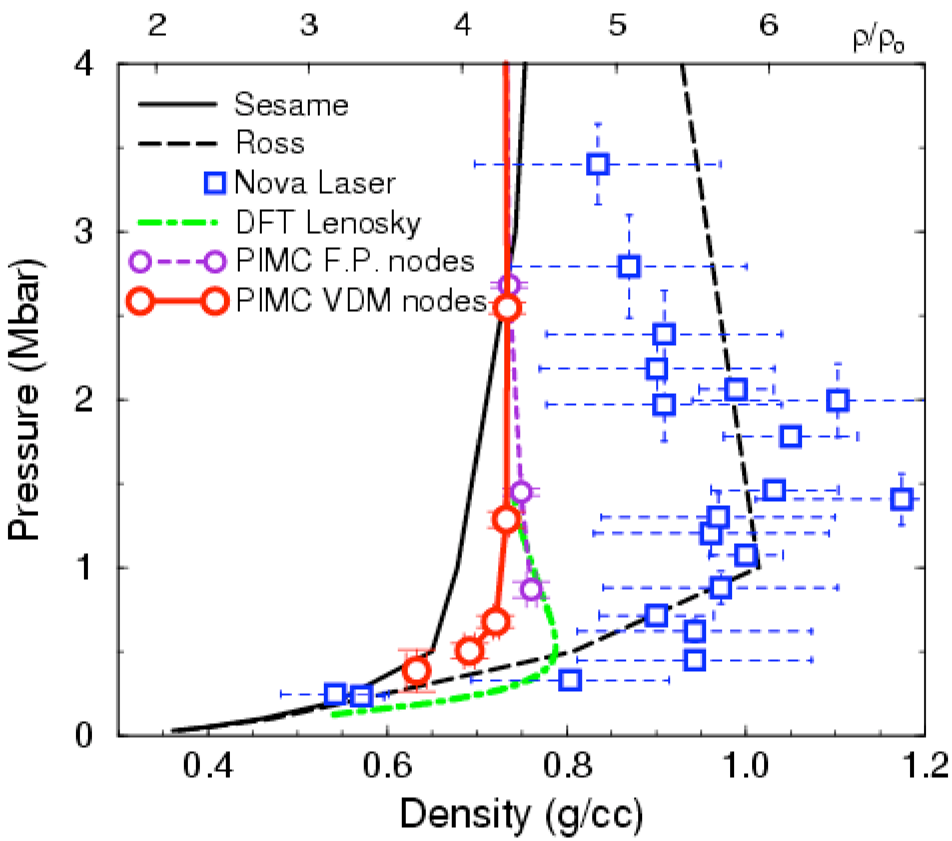
What does this imply for the dissociation of molecules?

Are electronic excitations important?

Nova laser results predict a 50% higher compressiblity.

# Deuterium Hugoniot

**Path integral Monte Carlo results**



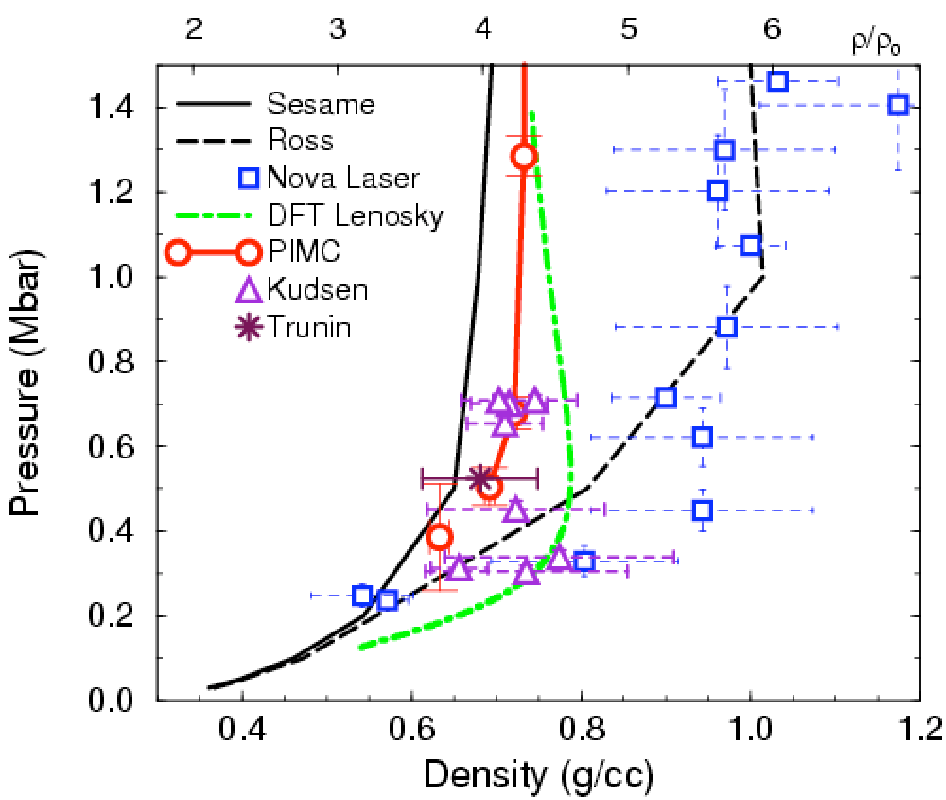

Militzer and Ceperley,
*Phys. Rev. Lett.* 85 (2000) 1890.
*Phys. Rev. Lett.* 87 (2001) 275502

- Accuracy increases with T
- Small size dependence
- Comparison of VDM and free particle nodes

Discrepancy:
E/N = 3 eV
PV/N=-2 eV

Good agreement between all *ab initio* methods.

# PIMC predicts low compressibility and agrees with more recent experiments




Militzer, Ceperley *et al.*
*Phys. Rev. Lett.* **85** (2000) 1890.
*Phys. Rev. Lett.* **87** (2001) 275502.

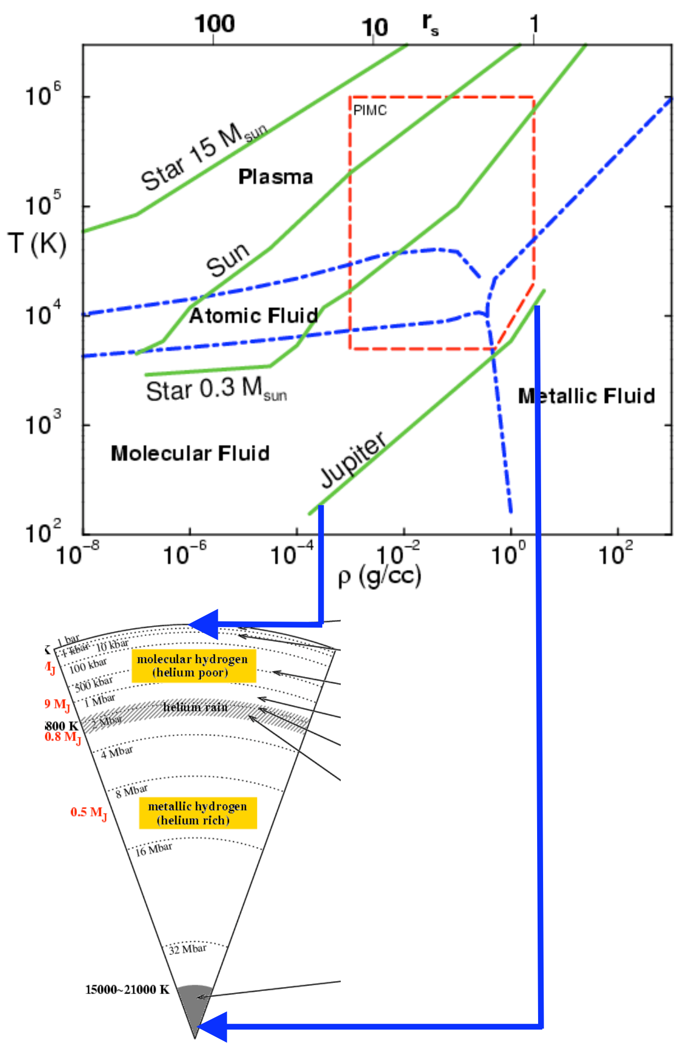
- Predict low compressibility!

Good agreement with:

- Magnetic shocks waves
  [Knudson *et al.*, PRL **87** (2001) 225501]
- Spherical converging shock waves
  [Belov et al, Boriskov et al.]
- DFT results (e.g. Bonev et al.)

Recent measurements agree reasonably well with first principle methods but need to be verified.

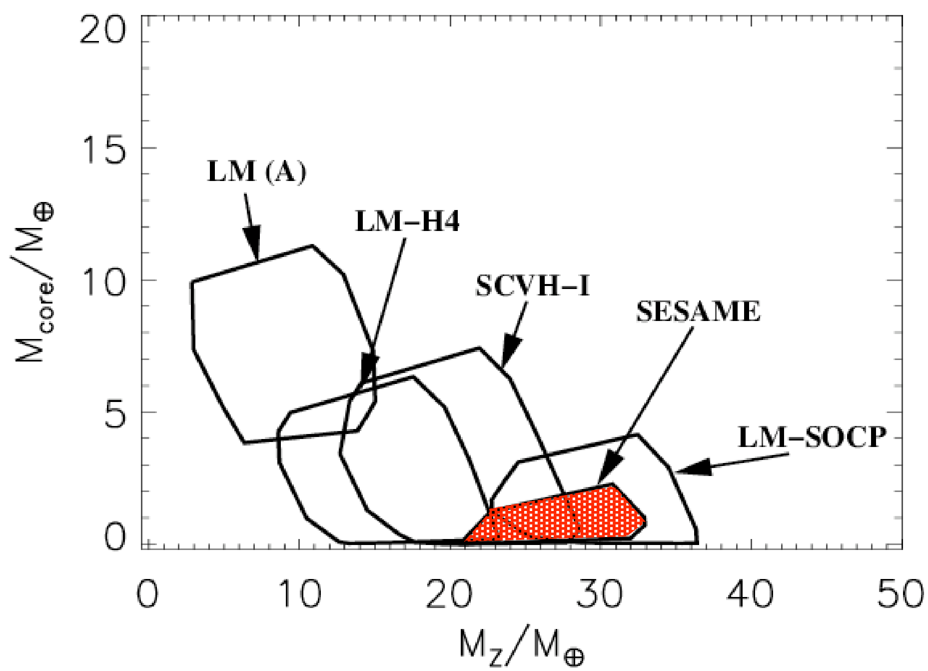
# T. Guillot's model: Uncertainties in EOS do not allow to determine if Jupiter has a rocky core




T. Guillot's three layer model is based on

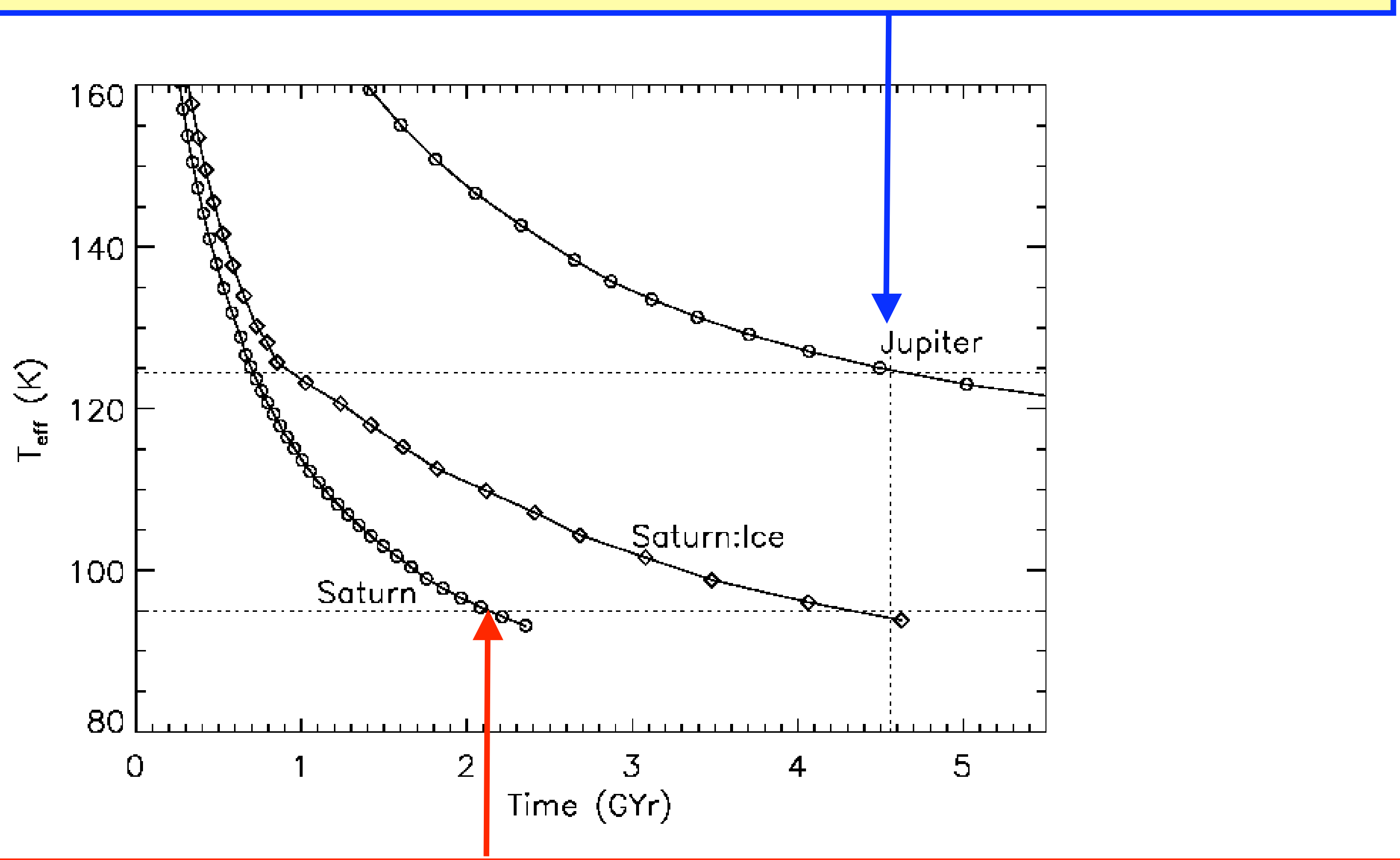
1) Hydrogen-helium EOS
2) Surface composition
3) Gravitational moments inferred from fly-by trajectories (Cassini mission)

Parameters like core mass or amount of heavier elements "Z" cannot be constraint well.



# J. Fortney & W. Hubbard model the evolution of Jupiter and Saturn [Icarus, 2003]

Jupiter's cooling rate is in agreement with model predictions




Model for Saturn consistently predict too fast cooling rates (by ~2 Gyrs)

# Predictions for Future Shock Experiments

- Repeat laser and magnetic shock experiments for helium. Both technique should reach of the regime of 5-fold compression. Can our prediction be verified?
- This could reveal any bias in either technique and help us understand the hydrogen results.
- Study electronic excitations and precompressed samples
- Future calculations: Improved models for Jovian planets:
  1) Do Jupiter has a core?
  2) Why is a too high cooling rate for Saturn predicted?
  3) Detect phase separation of H and He

**http://militzer.gl.ciw.edu**