Improving simulations of warm dense matter by developing thermal density functional theory

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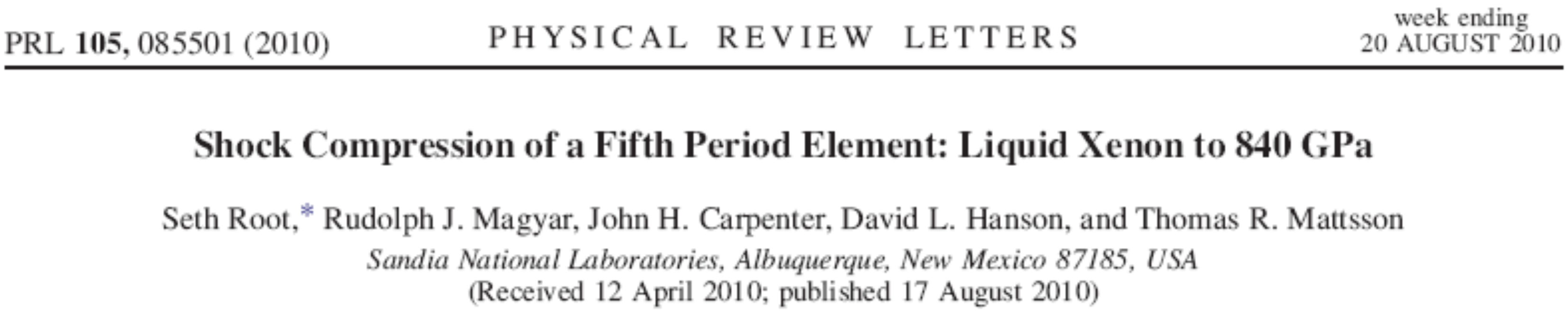
http://dft.uci.edu



PRL **105,** 085501 (2010) PHYSICAL REVIEW LETTERS week ending 20 AUGUST 2010

Shock Compression of a Fifth Period Element: Liquid Xenon to 840 GPa

Seth Root,* Rudolph J. Magyar, John H. Carpenter, David L. Hanson, and Thomas R. Mattsson

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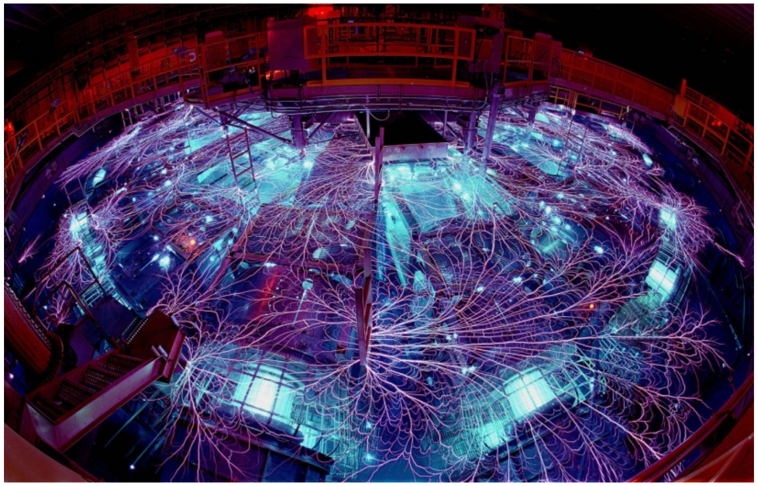
(Received 12 April 2010; published 17 August 2010)

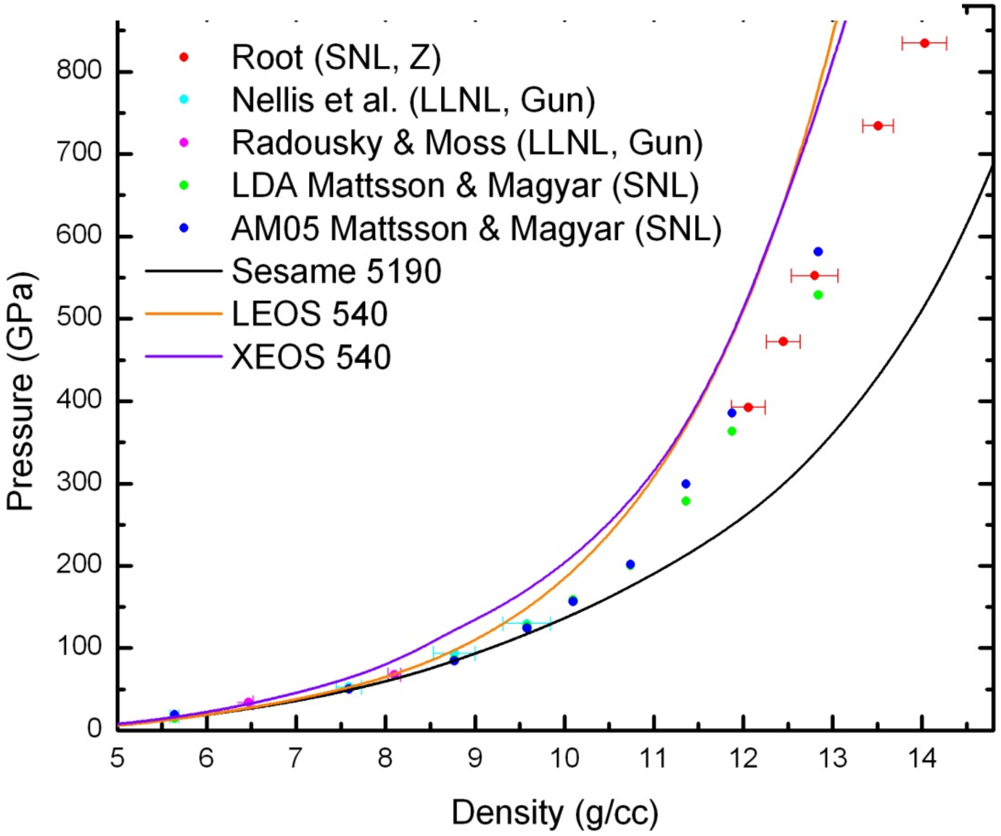


Z-pinch Pulsed Power System

- **Millions of amperes for less than 100 nanoseconds**
- **Peak temperature 3.7 GK or 6.6 billion °F, a world record**
- **Propelled small plates at 34 km/sec, 4x faster than a speeding bullet.**
- **Pressures 70,000 to 120,000 atm (7 to 12 Gpa).**

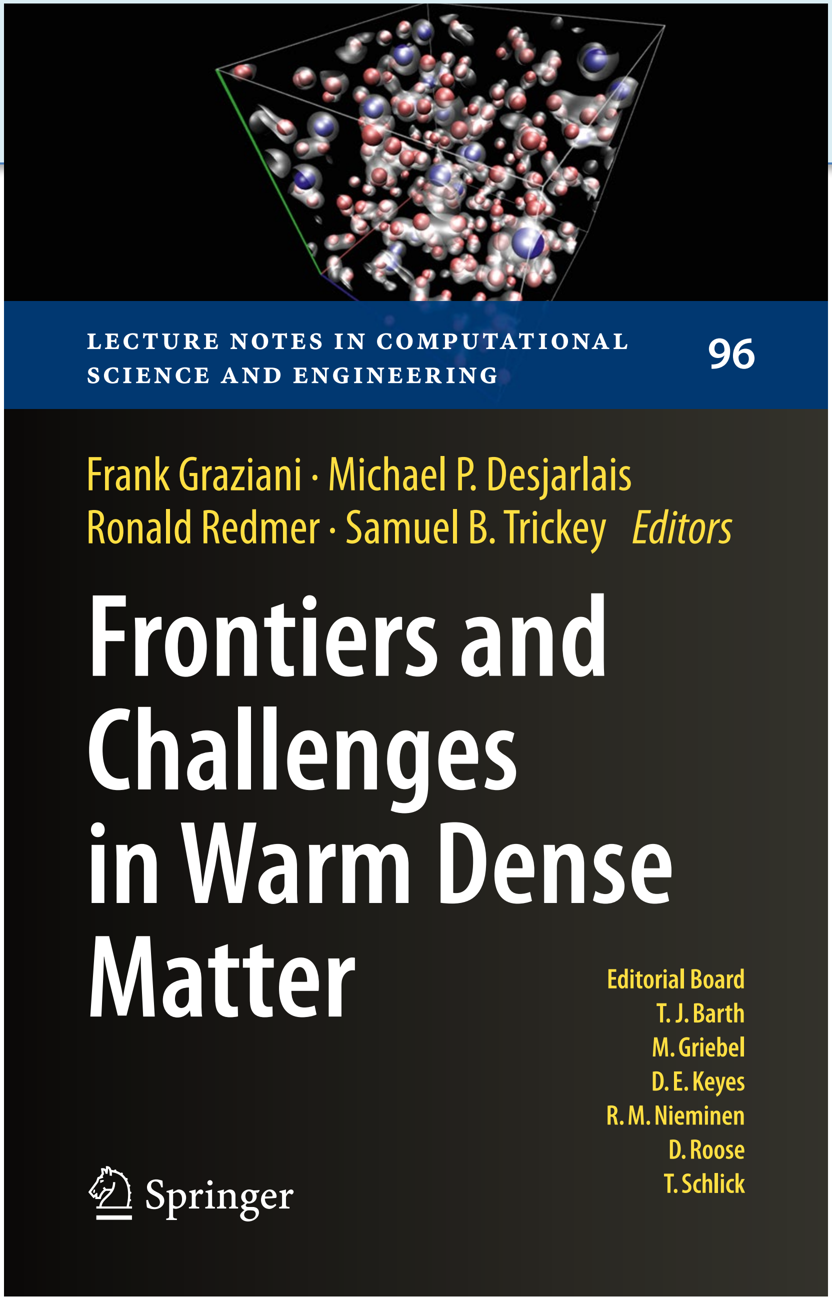
DFT-MD

- **Move classical nuclei in thermal quantum electrons**
- **VASP code (Georg Kresse, Vienna, Austria)**
- **World's tenth fastest computer**



Liquid Xenon Hugoniot

Submitted to PRL Root, Magyar, Carpenter, Hanson, Mattsson (2010).
DFT first published: Magyar and Mattsson CP1195, Shock Compression of Condensed Matter, 797 (2009).



LECTURE NOTES IN COMPUTATIONAL SCIENCE AND ENGINEERING 96

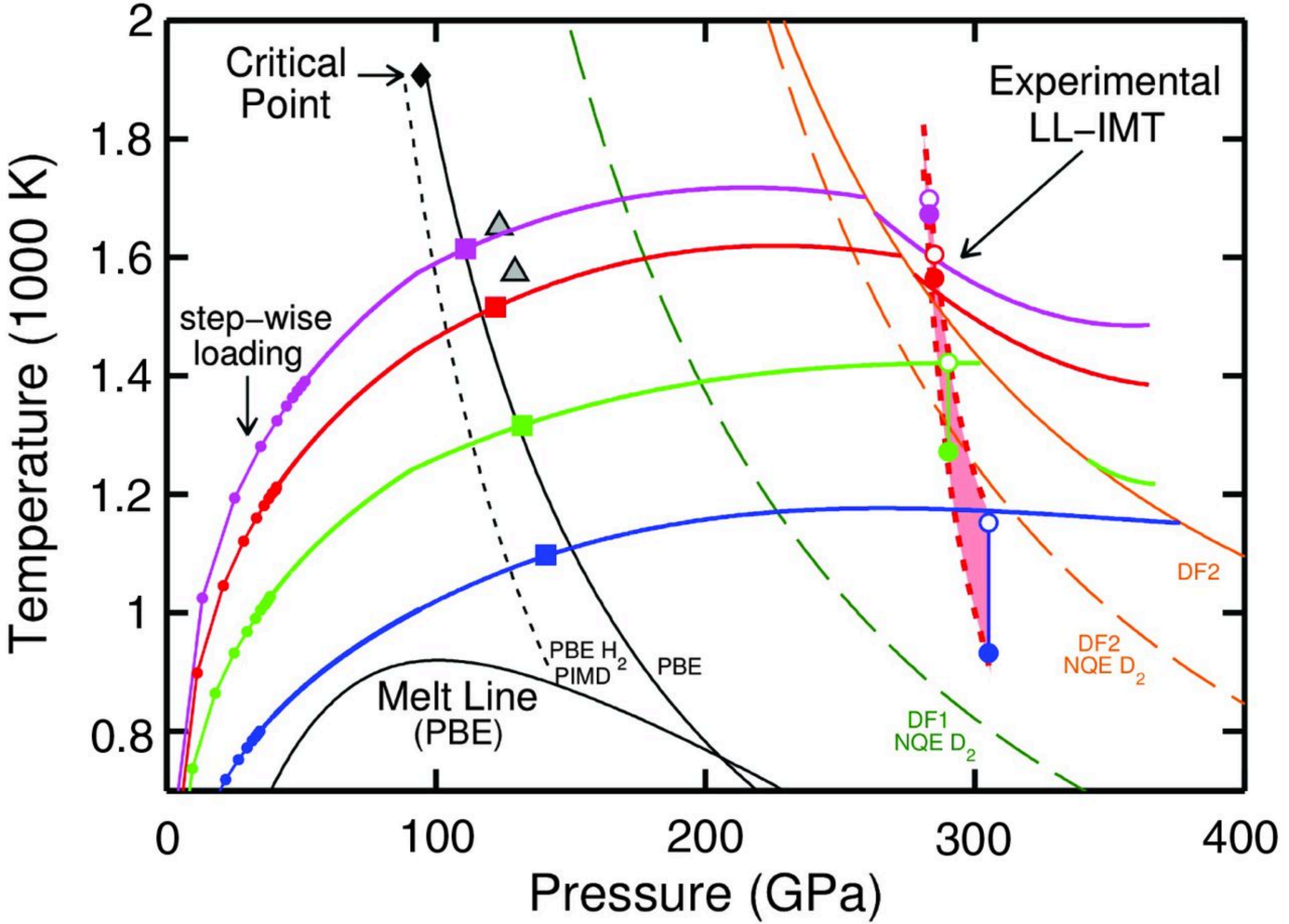
Frank Graziani · Michael P. Desjarlais
Ronald Redmer · Samuel B. Trickey *Editors*

Frontiers and Challenges in Warm Dense Matter

Springer

Deuterium phase diagram

Fig. 1 Deuterium PT diagram.



M. D. Knudson et al. Science 2015;348:1455-1460

Published by AAAS

Outline

- Relevant history of T=0 DFT
- Quantum MD: Thermal DFT and beyond
- Ways to attack problem at T=0
  - Exact conditions
  - Accurate calculations
- New results
  - Scaling relations and entropy formula
  - Hubbard model
  - Excitations in linear response
- Outlook

The electronic structure problem

- Use atomic units
- Born-Oppenheimer approximation
- All non-relativistic (but added back in)
- Wavefunctions antisymmetric and normalized
- Only discuss ground-state electronic problem here, but many variations.

Hamiltonian for N electrons in the presence of external potential $v(\mathbf{r})$:

$$\hat{H} = \hat{T} + \hat{V}_{\rm ee} + \hat{V},$$

where the kinetic and elec-elec repulsion energies are

$$\hat{T} = -\frac{1}{2}\sum_{i=1}^{N}\nabla_i^2, \qquad \hat{V}_{\rm ee} = \frac{1}{2}\sum_{i=1}^{N}\sum_{j\neq i}^{N}\frac{1}{|\mathbf{r}_i - \mathbf{r}_j|},$$

and difference between systems is N and the one-body potential

$$\hat{V} = \sum_{i=1}^{N} v(\mathbf{r}_i)$$

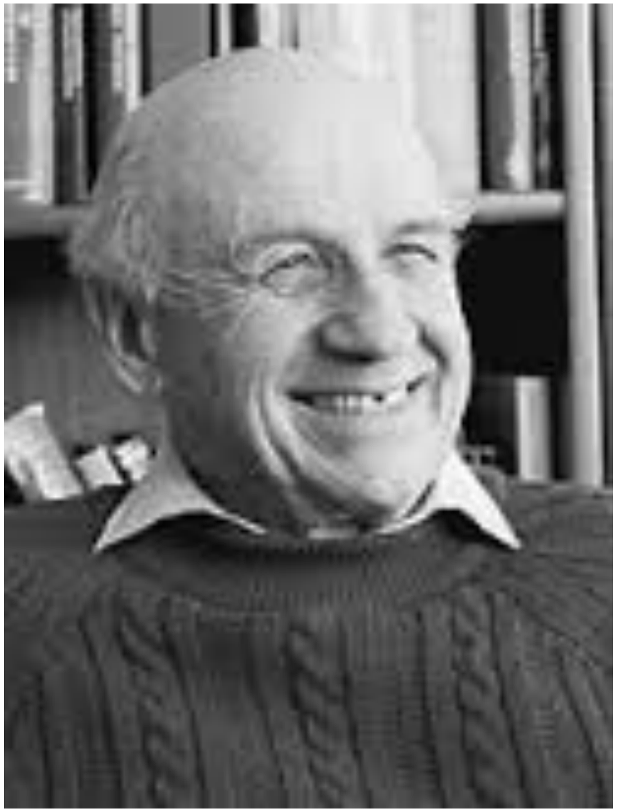
Often $v(\mathbf{r})$ is electron-nucleus attraction

$$v(\mathbf{r}) = -\sum_{\alpha}\frac{Z_\alpha}{|\mathbf{r} - \mathbf{R}_\alpha|}$$

where α runs over all nuclei, plus weak applied $\mathbf{E}$ and $\mathbf{B}$ fields.

$$\{\hat{T} + \hat{V}_{\rm ee} + \hat{V}\}\,\Psi = E\,\Psi, \qquad E = \min_{\Psi}\langle\Psi|\hat{T} + \hat{V}_{\rm ee} + \hat{V}|\Psi\rangle$$

Walter Kohn (1923-2016)

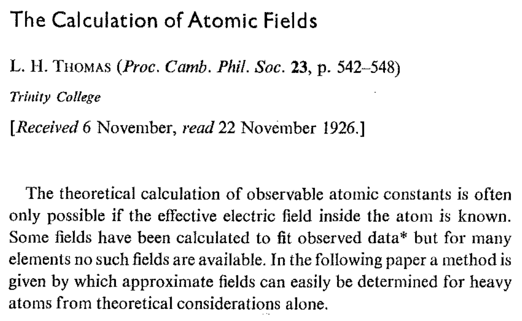


Timeline of ground-state electronic DFT

- 1926/27: Thomas-Fermi theory (stone-age)
- 1964/65: Medieval period
  - Hohenberg-Kohn theorems
  - Kohn-Sham equations
  - Local density approximation for $E_{XC}[n]$
  - Widely adopted in solid-state physics
- 1993: Modern era
  - Chemists show DFT with GGA/hybrids usefully accurate for thermochemistry
  - 1998 Nobel prize in chemistry to Kohn and Pople

Thomas/Fermi Theory 1927

- Derived in 1926 without Schrodinger eqn.



The Calculation of Atomic Fields

L. H. THOMAS (*Proc. Camb. Phil. Soc.* **23**, p. 542–548)

Trinity College

[*Received* 6 November, *read* 22 November 1926.]

The theoretical calculation of observable atomic constants is often only possible if the effective electric field inside the atom is known. Some fields have been calculated to fit observed data* but for many elements no such fields are available. In the following paper a method is given by which approximate fields can easily be determined for heavy atoms from theoretical considerations alone.

- Thomas-Fermi Theory (TF):
  - $T \approx T^{TF}$
  - $V_{ee} \approx U$ = Hartree energy
  - $V = \int d\mathbf{r}\, \mathbf{n}(\mathbf{r})\, v(\mathbf{r})$
  - $E_0 = T + V_{ee} + V$
  - Minimize $E_0[n]$ for fixed N

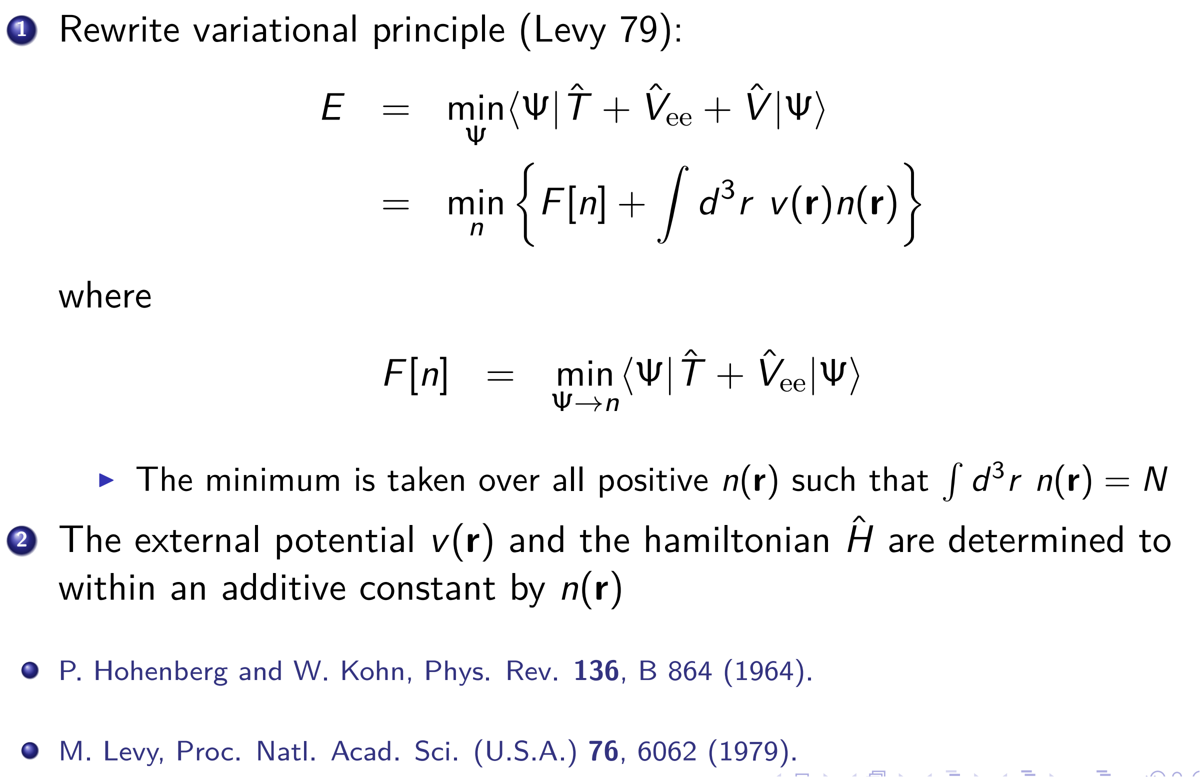
$$T_s^{loc} = \frac{3(3\pi)^{2/3}}{10} \int d^3r\, n^{5/3}(r)$$

$$U = \frac{1}{2} \int d^3r \int d^3r' \frac{n(r)n(r')}{|r - r'|}$$

- Properties:
  - Typical error of order 10%
  - Teller's unbinding theorem: Molecules don't bind.

HK theorem (1964)

- Makes TF an approximation to an exact theory
- Can find both ground-state density and energy via Euler equation



1. Rewrite variational principle (Levy 79):

$$
\begin{aligned}
E &= \min_{\Psi} \langle \Psi | \hat{T} + \hat{V}_{\mathrm{ee}} + \hat{V} | \Psi \rangle \\
&= \min_{n} \left\{ F[n] + \int d^3r \; v(\mathbf{r}) n(\mathbf{r}) \right\}
\end{aligned}
$$

where

$$
F[n] = \min_{\Psi \to n} \langle \Psi | \hat{T} + \hat{V}_{\mathrm{ee}} | \Psi \rangle
$$

   - ▸ The minimum is taken over all positive $n(\mathbf{r})$ such that $\int d^3r \; n(\mathbf{r}) = N$

2. The external potential $v(\mathbf{r})$ and the hamiltonian $\hat{H}$ are determined to within an additive constant by $n(\mathbf{r})$

- P. Hohenberg and W. Kohn, Phys. Rev. **136**, B 864 (1964).
- M. Levy, Proc. Natl. Acad. Sci. (U.S.A.) **76**, 6062 (1979).

KS equations (1965)

Define *fictitious* non-interacting electrons satisfying:

$$\left\{-\frac{1}{2}\nabla^2 + v_{\rm S}(\mathbf{r})\right\}\phi_j(\mathbf{r}) = \epsilon_j\phi_j(\mathbf{r}), \qquad \sum_{j=1}^{N}|\phi_j(\mathbf{r})|^2 = n(\mathbf{r}).$$

where $v_{\rm S}(\mathbf{r})$ is *defined* to yield $n(\mathbf{r})$.

Define $T_{\rm S}$ as the kinetic energy of the KS electrons, U as their Hartree energy and

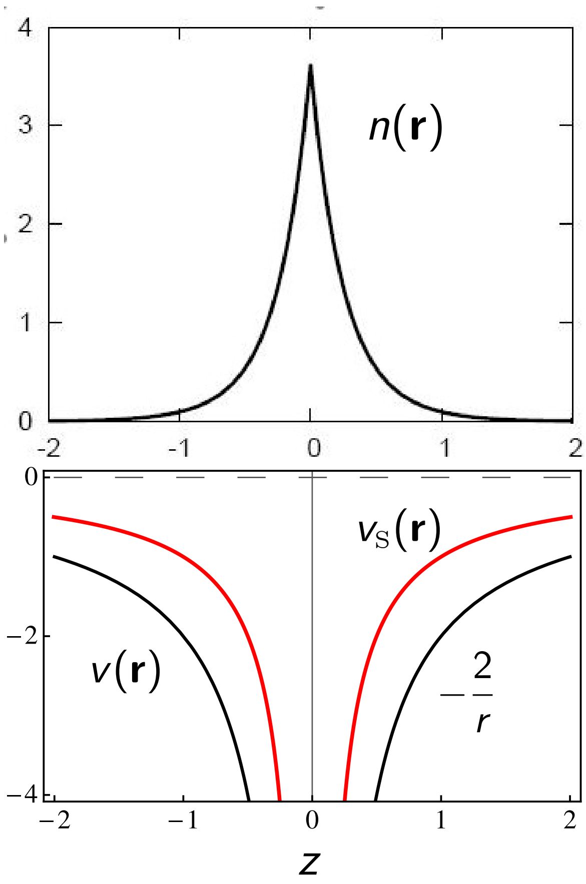
$$T + V_{\rm ee} = T_{\rm S} + U + E_{\rm XC}$$

the remainder is the exchange-correlation energy.

Most important result of exact DFT:

$$v_{\rm S}(\mathbf{r}) = v(\mathbf{r}) + \int d^3r\,\frac{n(\mathbf{r}')}{|\mathbf{r}-\mathbf{r}'|} + v_{\rm XC}[n](\mathbf{r}), \qquad v_{\rm XC}(\mathbf{r}) = \frac{\delta E_{\rm XC}}{\delta n(\mathbf{r})}$$

Knowing $E_{\rm XC}[n]$ gives closed set of self-consistent equations.



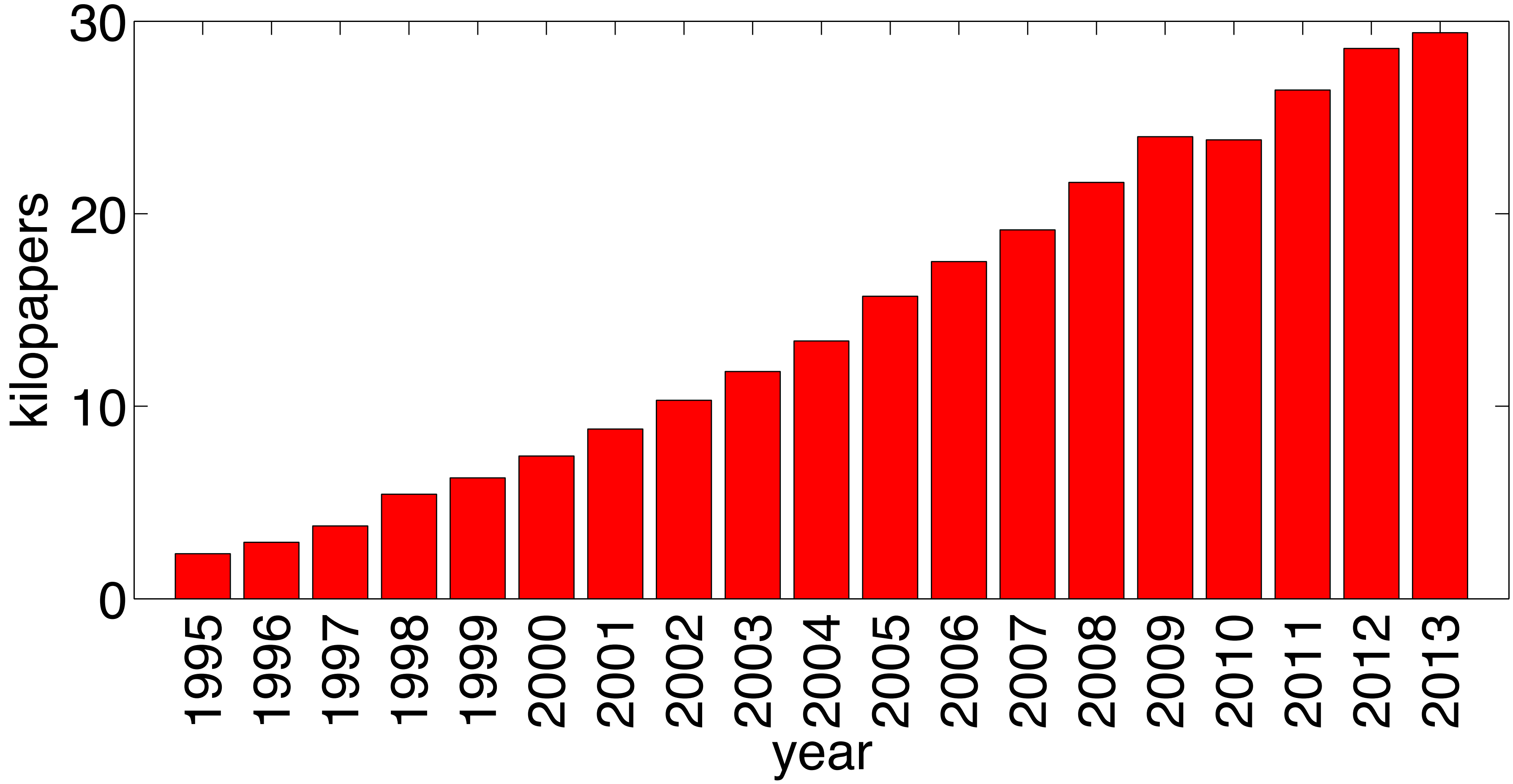
Today's commonly-used functionals

- Local density approximation (LDA) $E_X^{\text{LDA}}[n] = A_X \int d^3r \; n^{4/3}(\mathbf{r})$
  - Uses only n(**r**) at a point.

$$A_X = -(3/4)(3/\pi)^{1/3} = -0.738.$$

- Generalized gradient approx (GGA)
  - Uses both n(**r**) and |∇n(**r**)|
  - Should be more accurate, corrects overbinding of LDA
  - Examples are PBE and BLYP
- Hybrid:
  - Mixes some fraction of HF
  - Examples are B3LYP and PBE0

DFT papers



DFT: A Theory Full of Holes, Aurora Pribram-Jones, David A. Gross, Kieron Burke, Annual Review of Physical Chemistry (2014).

Things to know about ground-state DFT

- In ground-state DFT, only ever care about E as a function of nuclear coordinates.
- Formally, all other objects (eigenvalues, orbitals) not meaningful. Practically, they are often treated as physical.
- Knowledge of *exact* $E_{XC}[n]$ does *not* yield other properties (e.g. excitations) except what you can get from GS densities.
- Goal of modern DFT: Useful accuracy for energy differences in generic situations.

Utility of modern DFT

- DFT useful when a large number of people are solving the `same' problem over and over.
- Modern DFT is most useful *after* the physics is known.
- Modern-era produced improved energetics by an order-of-magnitude: vital for chemistry and materials science.
- My goal: To ensure same performance level for WDM

Systematic approach to DFT approximations

- How can dumb little formulas be so successful in solving the many-body problem?
- Success of local density approximation is via coarse-graining of space. Uses principle of locality.
- In fact, each component (T_s,E_x,E_c) becomes relatively exact in certain, large *N*, semiclassical limit.
- GGA's are our best attempt to get leading corrections for Coulombic systems.
- Corrections to Thomas-Fermi Densities at Turning Points and Beyond Raphael F. Ribeiro, Donghyung Lee, Attila Cangi, Peter Elliott, Kieron Burke,*Phys. Rev. Lett.* **114**, 050401 (2015) Almost exact exchange at almost no computational cost in electronic structure calculations Peter Elliot, Attila Cangi, Stefano Pittalis, E.K.U. Gross, Kieron Burke, *Phys. Rev. A (accepted)* (2015) Potential functionals versus density functionals Attila Cangi, E. K. U. Gross, Kieron Burke, *Phys. Rev. A* **88**, 062505 (2013). Electronic Structure via Potential Functional Approximations Attila Cangi, Donghyung Lee, Peter Elliott, Kieron Burke, E. K. U. Gross, *Phys. Rev. Lett.***106**, 236404 (2011) Leading corrections to local approximations Attila Cangi, Donghyung Lee, Peter Elliott, Kieron Burke, *Phys. Rev. B* **81**, 235128 (2010)…

Overview of ALL TDDFT

1. General Time-dependent Density Functional Theory

- Any e$^-$ system subjected to any $v_{\text{ext}}(\mathbf{r}t)$
- Only unknown: $v_{\text{XC}}[\rho](\mathbf{r}t)$
- Treat atoms and molecules in INTENSE laser fields

2. TDDFT linear response to weak fields

- Linear response: $\delta\rho(\mathbf{r}t) = \int d^3r' \int dt' \, \chi(\mathbf{r}\mathbf{r}', t-t') \, \delta v_{\text{ext}}(\mathbf{r}'t')$
- Only unknown: $v_{\text{XC}}(\mathbf{r}t)$ near ground state

$$v_{\text{XC}}[\rho_0 + \delta\rho](\mathbf{r}\omega) = v_{\text{XC}}[\rho_0](\mathbf{r}) + \int d^3r' \, f_{\text{XC}}[\rho_0](\mathbf{r}\mathbf{r}'\omega) \, \delta\rho(\mathbf{r}'\omega)$$

- Treat electronic excitations in atoms + molecules + solids

3. Ground-state Energy from TDDFT

- Fluctuation-dissipation theorem: E_{XC} from susceptibility (RPA)
- Van der Waals; seamless dissociation

Basic approximation: ALDA $v_{\text{XC}}^{\text{unif}}(\rho(\mathbf{r}t))$

Importance of TDDFT

- Most success of TDDFT is in linear response regime.
- No practical general purpose scheme to go beyond Born-Oppenheimer
- Hard to see how to develop accurate functionals for a few electrons in strong laser fields: Must surely be orbital-dependent.
- TDDFT turns KS eigenvalues into zero-order approximations to optical excitations.

Warm dense matter

- Thermal DFT began with Mermin generalization of HK theorem (1965).
- Yields equilibrium properties analogous to how ground-state DFT works.
- Construct MKS equations at finite T.
- Does not produce dynamic response
- Standard QMD for equilibrium ignores thermal corrections to XC
- QMD for transport ignores time-dependent XC

Many years of development

- Much development in plasma physics
  - Eg book by Ichimaru
- Thermal homogeneous electron gas
  - Various many-body calculations, Dharma-Wardana and Perrot parametrization
  - Eg ***XC potentials for electron-ion systems at finite temperature*,**Perrot, Francois and Dharma-wardana, M. W. C, PRA 1984
- More recently: CHNC, etc.
- But older work not at GGA level

Recent realistic QMD calculations

- Run VASP with thermal occupations
- Find self-consistent solution using, e.g. GGA or hybrid or meta-GGA
- Also calculate response properties like conductivity from Kubo response on MKS orbitals
- Always makes ground-state approximation (GSA) for XC

Two basic questions

- Warm XC equilibrium question:
  - How important are thermal XC corrections to equilibrium? These are ignored in QMD
  - Errors in equil free energy, density, orbitals.
- Warm XC non-equilibrium question:
  - How can we put in non-equilibrium effects?
  - Two distinct aspects
    - Linear response, yielding transport properties
    - Strong perturbations, e.g., stopping or strong radiation
- References:
  - Four recent papers by Pribram-Jones, Grabowski, Smith, and KB

Equilibrium

- Mermin theorem (Levy constrained search)

$$A = \min_{n}\left(F[n] + \int d^3r\,(v(\mathbf{r}) - \mu)\right)$$

$$F[n] = \min_{\Gamma\to n} Tr\left\{(\hat{T} + \hat{V}_{\rm ee} - \tau\hat{S})\Gamma\right\}$$

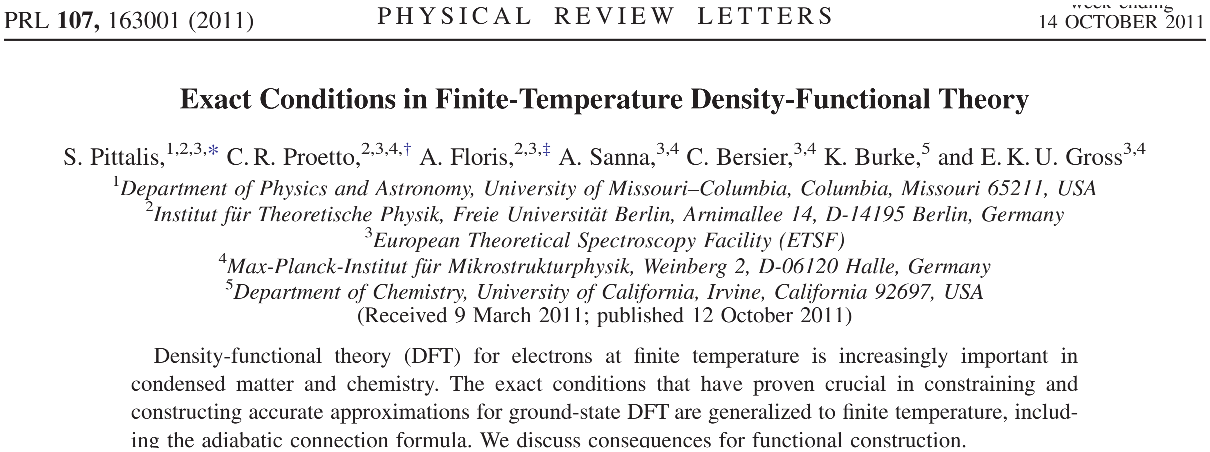
- Mermin-KS equations:

$$\left\{-\frac{1}{2}\nabla^2 + v_{\rm S}^{\tau}(\mathbf{r})\right\}\phi_i^{\tau}(\mathbf{r}) = \epsilon_i^{\tau}\,\phi_i^{\tau}(\mathbf{r})$$

$$v_{\rm S}^{\tau}[n](\mathbf{r}) = v(\mathbf{r}) + v_{\rm H}[n](\mathbf{r}) + v_{\rm XC}^{\tau}[n](\mathbf{r}),$$

$$n^{\tau}(\mathbf{r}) = \sum_i f_i^{\tau}\,|\phi_i^{\tau}(\mathbf{r})|^2.$$

Earlier work on fundamentals



PRL **107,** 163001 (2011) PHYSICAL REVIEW LETTERS 14 OCTOBER 2011

Exact Conditions in Finite-Temperature Density-Functional Theory

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(Received 9 March 2011; published 12 October 2011)

Density-functional theory (DFT) for electrons at finite temperature is increasingly important in condensed matter and chemistry. The exact conditions that have proven crucial in constraining and constructing accurate approximations for ground-state DFT are generalized to finite temperature, including the adiabatic connection formula. We discuss consequences for functional construction.

$$\Omega_{\mathrm{C}}^{\tau}[n] \leq 0, \qquad U_{\mathrm{C}}^{\tau}[n] \leq 0, \qquad K_{\mathrm{C}}^{\tau}[n] \geq 0,$$

$$F^{\tau,\lambda}[n] = \lambda^2 F^{\tau/\lambda^2}[n_{1/\lambda}],$$

$$\Omega_{\mathrm{XC}}^{\tau}[n] = \int_0^1 d\lambda\, U_{\mathrm{XC}}^{\tau}[n](\lambda),$$

Constructing thGGA

- Need
  - exact conditions to constrain functional
  - highly accurate calculations to compare with.
  - gradient expansion

- thLDA
  - XC for uniform gas roughly known for long time (but not used in modern QMD)
  - Recent interest means PRL each year on subject
  - Should not use in combo with GGA

Exact conditions

- Look like standard formulas, but really very different.
- For A_s and E_X, can be quite simple; much more subtle for correlation.
- E.g., found adiabatic connection formula can be written as

$$A^{\tau}_{\rm XC}[n] = \frac{\tau}{2}\int_{\tau}^{\infty}\frac{d\tau'}{\tau'^2}\,U^{\tau'}_{\rm XC}[n_{\sqrt{\tau'/\tau}}] \qquad n_\gamma(\mathbf{r}) = \gamma^3\, n(\gamma\mathbf{r})$$

- APJ and KB, arXiv:1509.03060

Exact conditions on entropy

- Use definition to show equality:

$$\frac{dF^\tau[n]}{d\tau} = -S^\tau[n]. \qquad F^\tau[n] = F^0[n] - \int_0^\tau d\tau' \, S^{\tau'}[n],$$

- Can also prove inequalities:

$$dS^\tau[n]/d\tau \ge 0. \qquad d^2F^\tau[n]/d\tau^2 \le 0. \qquad \frac{dT_{\mathrm{S}}^\tau[n]}{d\tau}, \frac{dS_{\mathrm{S}}^\tau[n]}{d\tau} \ge 0 \ge \frac{dF_{\mathrm{S}}^\tau[n]}{d\tau}, \frac{d^2F_{\mathrm{S}}^\tau[n]}{d\tau^2}$$

- For XC

$$\frac{dA^\tau_{\mathrm{XC}}[n]}{d\tau} = -S^\tau_{\mathrm{XC}}[n] \qquad A^\tau_{\mathrm{XC}}[n] = E_{\mathrm{XC}}[n] - \int_0^\tau d\tau' \, S^{\tau'}_{\mathrm{XC}}[n].$$

Use of exact conditions

- Automatically satisfied by LDA in MKS and by TF theory (because unif gas is a real WDM system)
- Can be used to check parametrizations of $a_{xc}(r_s,T)$ for unif gas
- Can be built-in to more advanced approximations, such as thGGA, constraining forms
- Can test other approximations against conditions
- Can think in terms of free energy, potential energy, or entropy alone (as all related).

Test of unif gas parametrization

- Note: This is unlikely to be an issue in any LDA calculation of a realistic material.

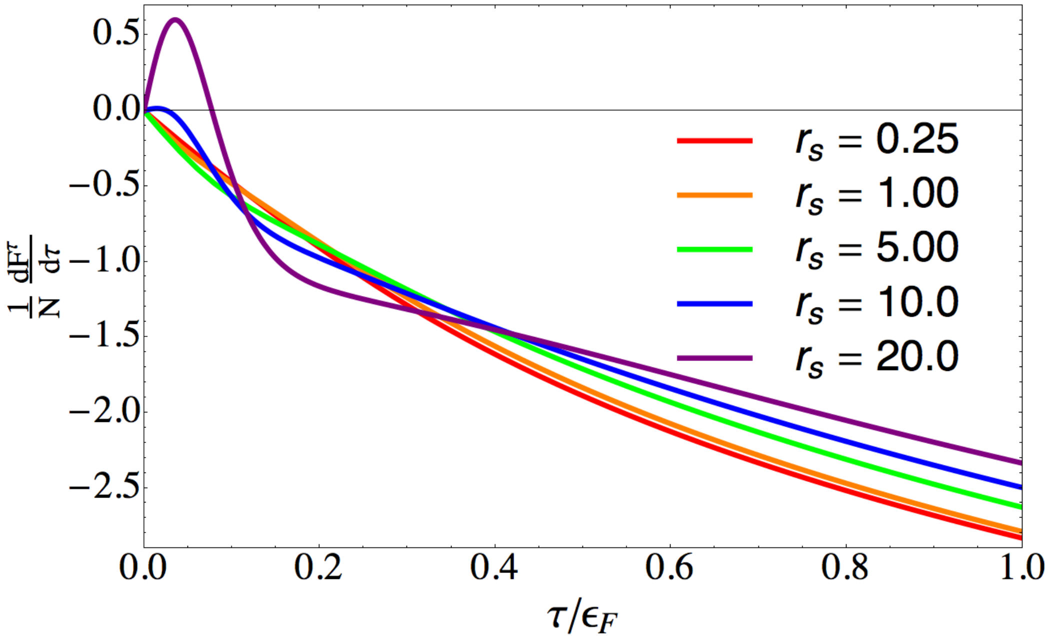
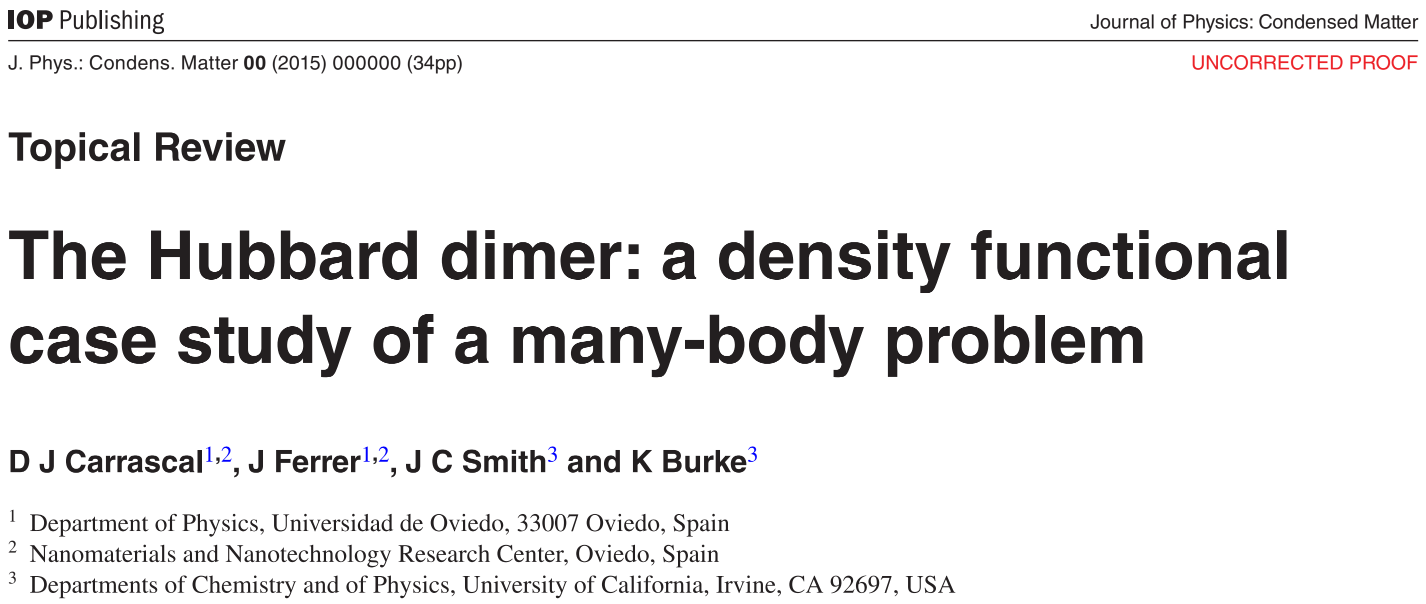


FIG. 2. Temperature dependence of the Mermin functional for spin-unpolarized uniform gas for several values of the Wigner-Seitz radius r_S, using the XC parametrization of Ref. [16], where ϵ_F is the Fermi energy.

Exact calculations of WDM

- Crucial part of functional construction: Testing accuracy and reliabilty
- Revolution in chemistry due to existing G2 data set in 1993
- Very difficult to achieve quantum chemical accuracy for correlation energies at finite T
- Even difficult to do H atom (since you must included all particle numbers)

DFT for Hubbard dimer



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Journal of Physics: Condensed Matter
J. Phys.: Condens. Matter **00** (2015) 000000 (34pp)
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Topical Review

The Hubbard dimer: a density functional case study of a many-body problem

D J Carrascal[1,2], J Ferrer[1,2], J C Smith[3] and K Burke[3]

[1] Department of Physics, Universidad de Oviedo, 33007 Oviedo, Spain
[2] Nanomaterials and Nanotechnology Research Center, Oviedo, Spain
[3] Departments of Chemistry and of Physics, University of California, Irvine, CA 92697, USA

$$\hat{H} = -t\sum_{\sigma}(\hat{c}^{\dagger}_{1\sigma}\hat{c}_{2\sigma} + h.c) + U\sum_{i}\hat{n}_{i\uparrow}\hat{n}_{i\downarrow} + \sum_{i} v_i\hat{n}_i$$

- Simplest possible model of simplest possible molecule with correlation, H_2.

Testing ground-state approximation

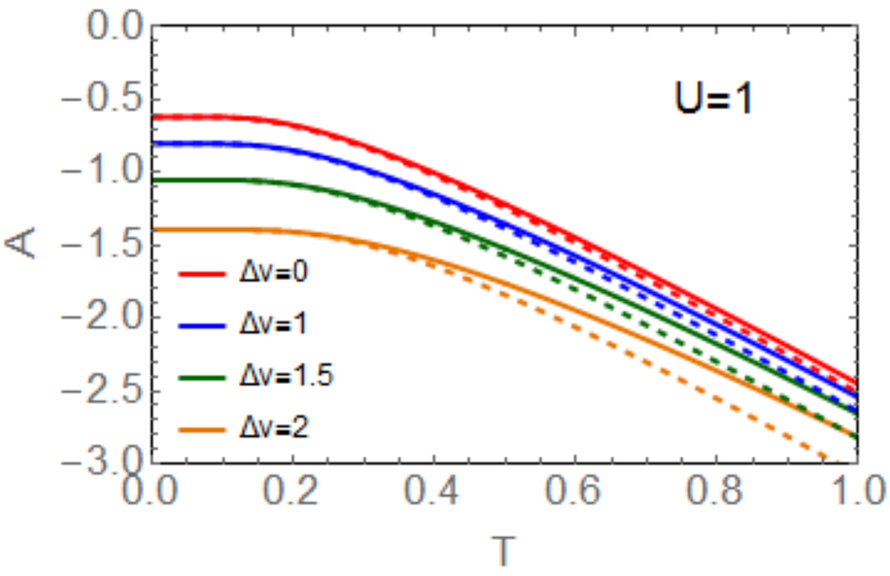
- Conditions chosen to mimic WDM
- T not too big
- U not too big
- All in units of 2t.

Justin Smith

Aurora Pribram-Jones

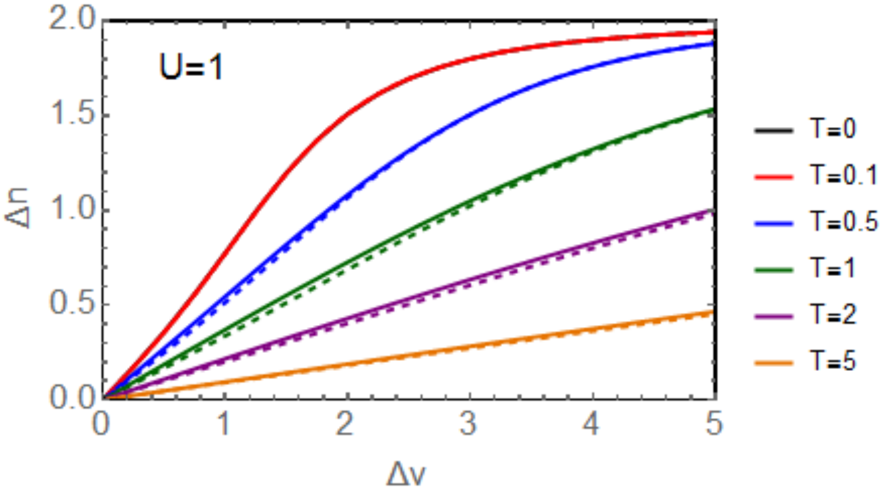
- JS,APJ,KB,
- arXiv:1509.03097

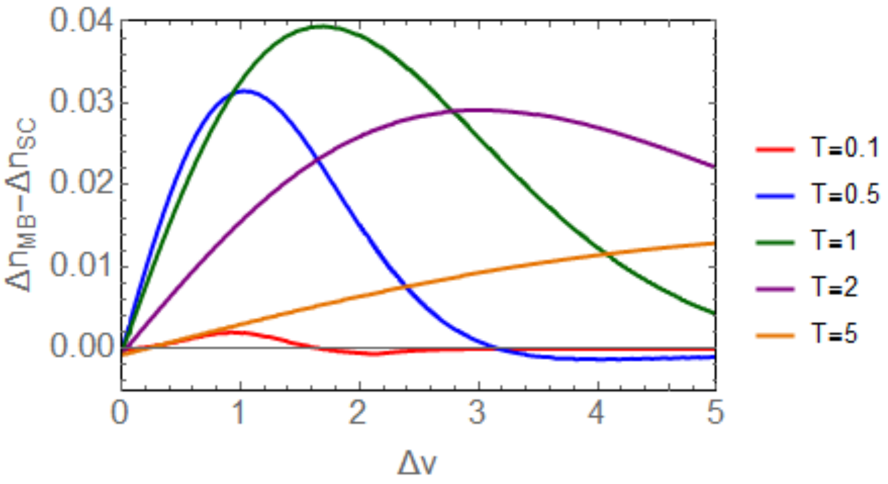
Free energy versus temperature



Solid lines: Exact free energy
Dashed lines: Solution of MKS with ground-state XC functional.

Density and GSA density





Exact conditions on entropy

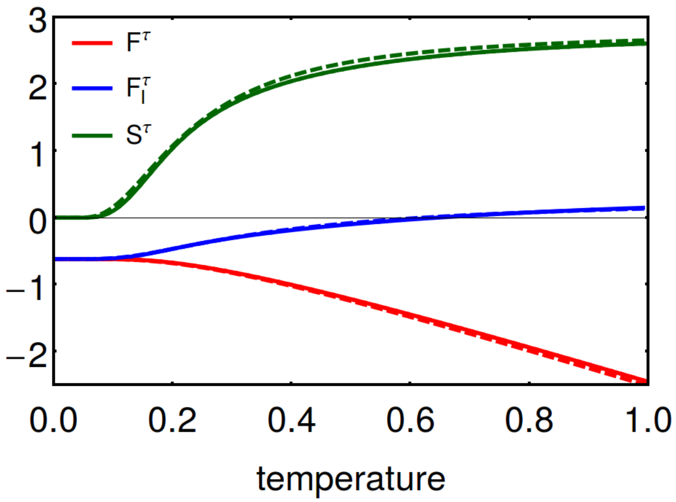


FIG. 1. Energy components for the Hubbard dimer in units of $2t$, where $U = 2t$ and $\Delta n = 0$: $F^{\tau}, F_{\mathrm{I}}^{\tau}, S^{\tau}$, both interacting (solid) and non-interacting (dashed).

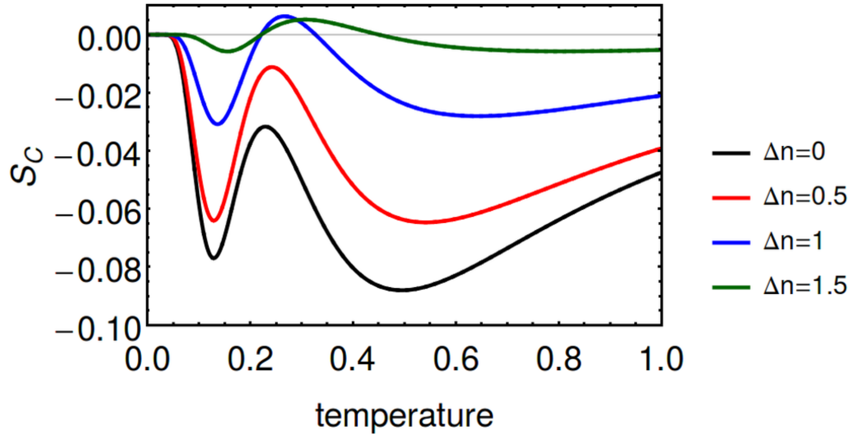


FIG. 3. Correlation entropy in the Hubbard dimer for several values of Δn as a function of temperature, in units of $2t$, where $U = 2t$.

- Note: Cannot use Hubbard dimer to test LDA and GGA XC approximations.

thTDDFT

- Many processes require thermal TDDFT
- E.g. stopping of a fast nucleus in matter
- But any description must involve coupling of electrons and nuclei, beyond Born-Oppenheimer and beyond Mermin functional.
- Many, many illegal calculations nonetheless.
- Aim: Less lofty goal
  - just linear response to weak time-dependent perturbation
  - Joule heating is 2nd order in perturbation, so temperature stays fixed
  - Yields corrections to conductivities in MKS calculations

Basic idea of proof

- Generalize van Leeuwen proof for linear response TDDFT to finite temperature.
- Start from non-degenerate ground state.
- Account for finite numbers of degeneracies in excited states.
- Avoids two problems with RG-style proofs:
  - Cusps in initial wavefunction at nuclei
  - Need to invoke boundary conditions

Thermal XC linear response

Thermal Density Functional Theory: Time-Dependent Linear Response and Approximate Functionals from the Fluctuation-Dissipation Theorem Aurora Pribram-Jones, Paul E. Grabowski, Kieron Burke, *Phys. Rev. Lett.* **116**, 233001 (2016)

$$\chi^\tau(12) = \chi_{\rm S}^\tau(12) + \int d3d4\, \chi_{\rm S}^\tau(13)\, f_{\rm HXC}^\tau(34)\chi^\tau(42)$$

$$A_{\rm XC}^\tau[n] = \frac{\tau}{2}\int_\tau^\infty \frac{d\tau'}{\tau'^2} \int \overline{d1d2}\, \{\Im\chi^\tau[n_\gamma](12) - n_\gamma(\mathbf{r})\delta(12)\}$$

$$\gamma = \sqrt{\tau'/\tau}.$$

New route to equil approximations

- Feed approximate kernels into thermal Gross-Kohn equation and get RPA with corrections:

$$f_{\mathrm{XC}}^{\tau,\mathrm{TALDA}}[n](\mathbf{r},\mathbf{r}',\omega) = \left.\frac{d^2 a_{\mathrm{XC}}^{\tau,\mathrm{unif}}(n)}{d^2 n}\right|_{n(\mathbf{r})} \delta(\mathbf{r}-\mathbf{r}'),$$

- Can test for uniform gas and Hubbard dimer
- Gives new approximations for $E_{\mathrm{XC}}(T)$

New book chapter

Warming Up Density Functional Theory

Justin C. Smith, Francisca Sagredo, and Kieron Burke

Abstract Density functional theory (DFT) has become the most popular approach to electronic structure across disciplines, especially in material and chemical sciences. Last year, at least 30,000 papers used DFT to make useful predictions or give insight into an enormous diversity of scientific problems, ranging from battery development to solar cell efficiency and far beyond. The success of this field has been driven by usefully accurate approximations based on known exact conditions and careful testing and validation. In the last decade, applications of DFT in a new area, warm dense matter, have exploded. DFT is revolutionizing simulations of warm dense matter including applications in controlled fusion, planetary interiors, and other areas of high energy density physics. Over the past decade or so, molecular dynamics calculations driven by modern density functional theory have played a crucial role in bringing chemical realism to these applications, often (but not always) with excellent agreement with experiment. This chapter summarizes recent work from our group on density functional theory at non-zero temperatures, which we call thermal DFT. We explain the relevance of this work in the context of warm dense matter, and the importance of quantum chemistry to this regime. We illustrate many basic concepts on a simple model system, the asymmetric Hubbard dimer.

arXiv:1701.00873

Conclusions

- Many successful applications of DFT for WDM, using ground-state XC in MKS equations
- Our group (and others) trying to further develop DFT to account for WDM effects
  - Many exact conditions on thermal XC functionals
  - First exact calculations of thermal XC (on model system)
  - Proof of linear response thTDDFT
  - Corrections to RPA for new thermal XC approx
- Funding
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To explore

- Construction of thPBE
- Accuracy of new method of finding approximations
- Testing new method against exact conditions
- Too many different possibilities for Hubbard model

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