Exact Conditions in Finite-Temperature DFT

Dr. Stefano Pittalis
Department of Chemistry
University of California, Irvine

Co-authors

Phys. Rev. Lett. 107, 163001 (2011)

- Dr. A. Floris
  King's College, London, U.K.
- Dr. A. Sanna
  Max-Planck Institute, Halle, Germany
- Dr. C. Bersier
  Max-Planck Institute, Halle, Germany
- Prof. C. Proetto
  Centro Atomico Bariloche, Argentina
- Prof. K. Burke
  University of California, Irvine
- Prof. E.K.U. Gross
  Max-Planck Institute, Halle, Germany

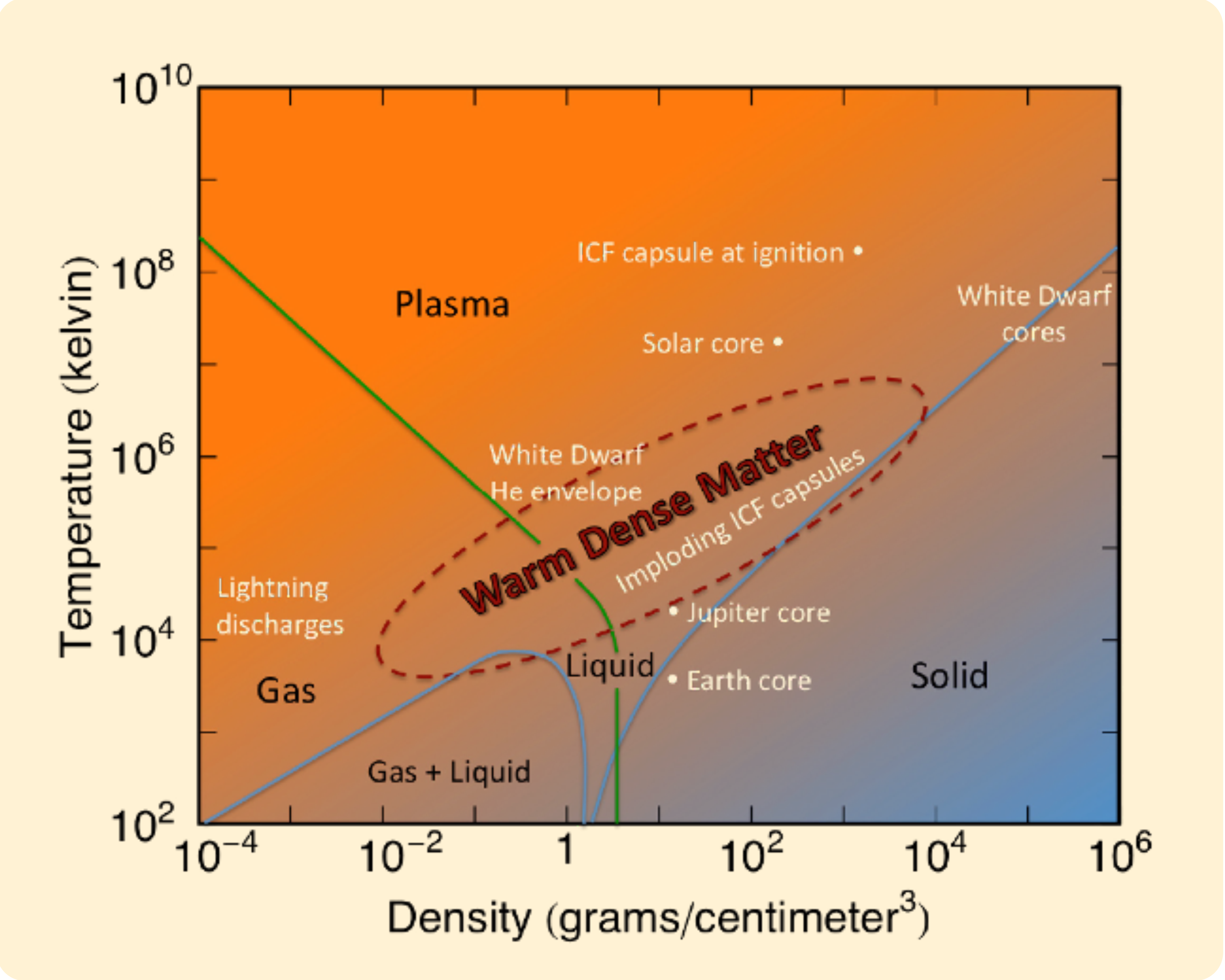
Outline

- Motivation
- Formal construction of finite-temperature (FT) density functionals (DFs)
- Some elementary facts
- Scaling in FT DF-Theory (FT-DFT)
- Conclusions and outlooks

Motivation

First-principle approach to determine thermodynamical properties of many-electron systems: universal, accurate, and practical!

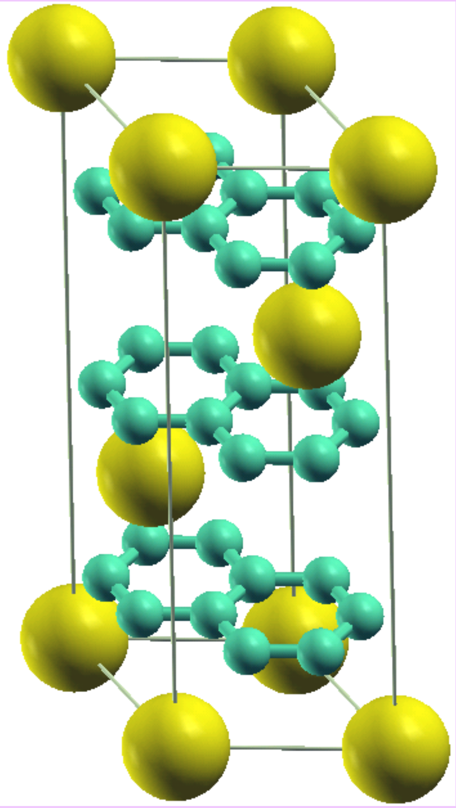
Warm Dense Matter



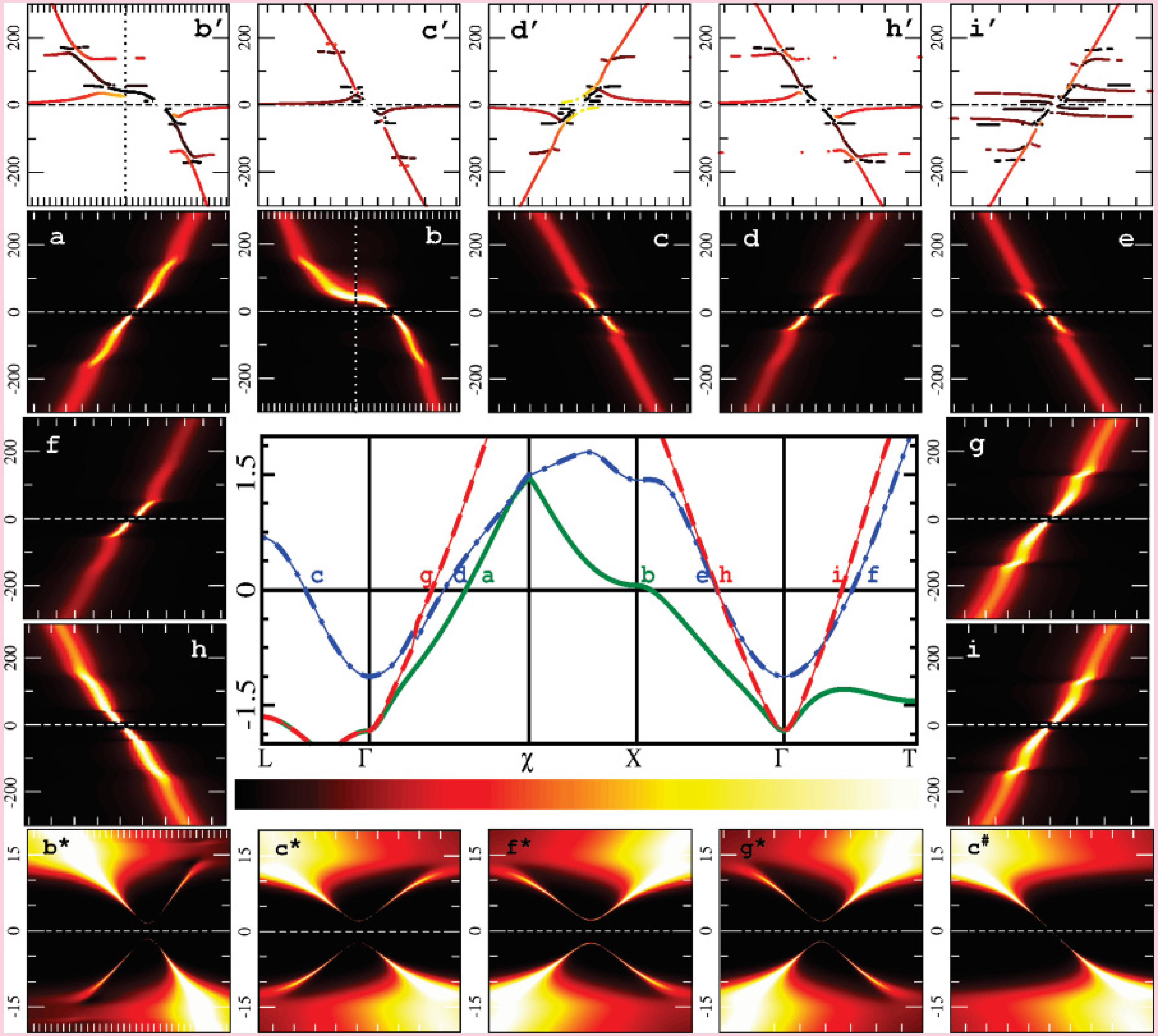
* *Diagram from:* *http://www.qtp.ufl.edu/ofdft/*

Superconductivity

System: CaC_6

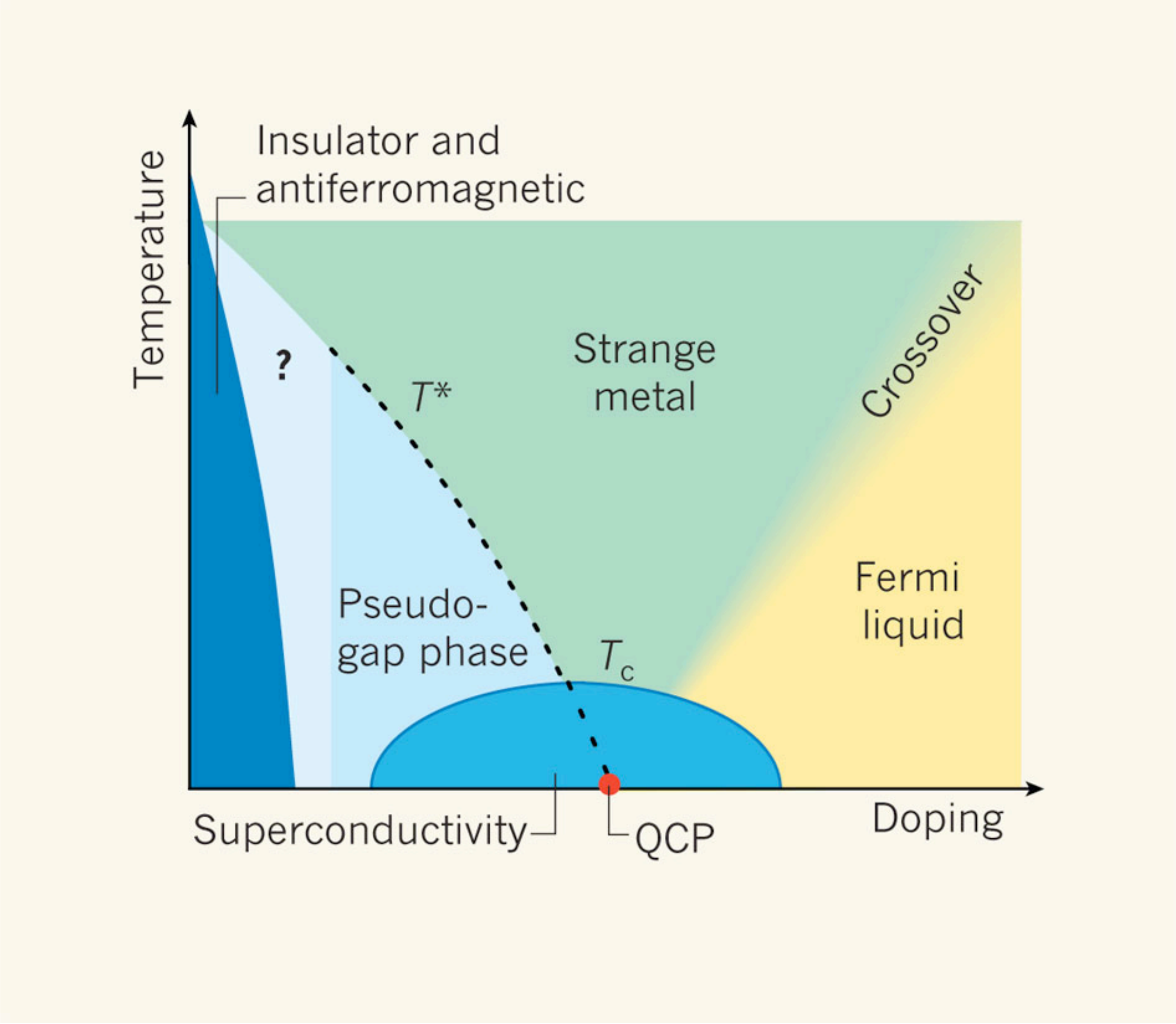


Sanna, Pittalis, Dewhurst, Monni, Sharma, Ummarino, Massidda, Gross, PRB (2012)



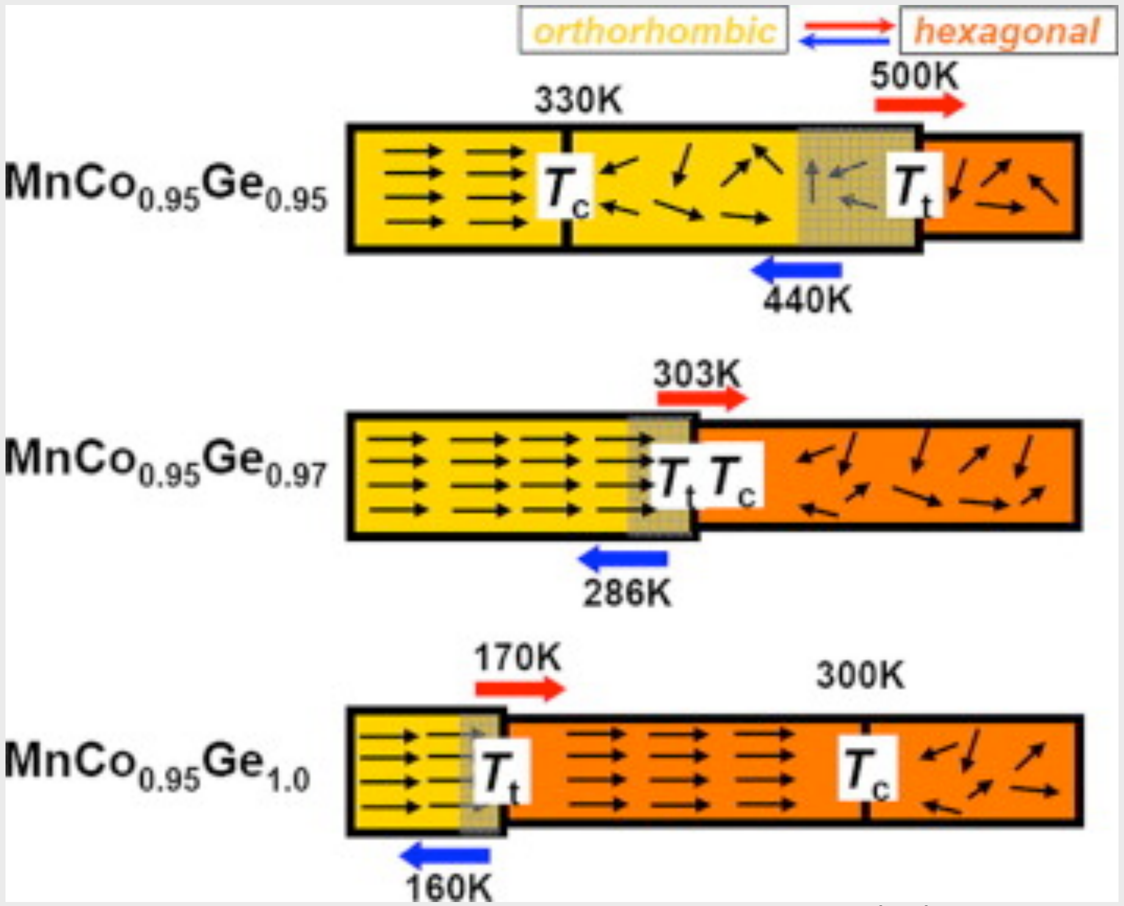
Results: “polaronic” spectral function

High-T_c Superconductors

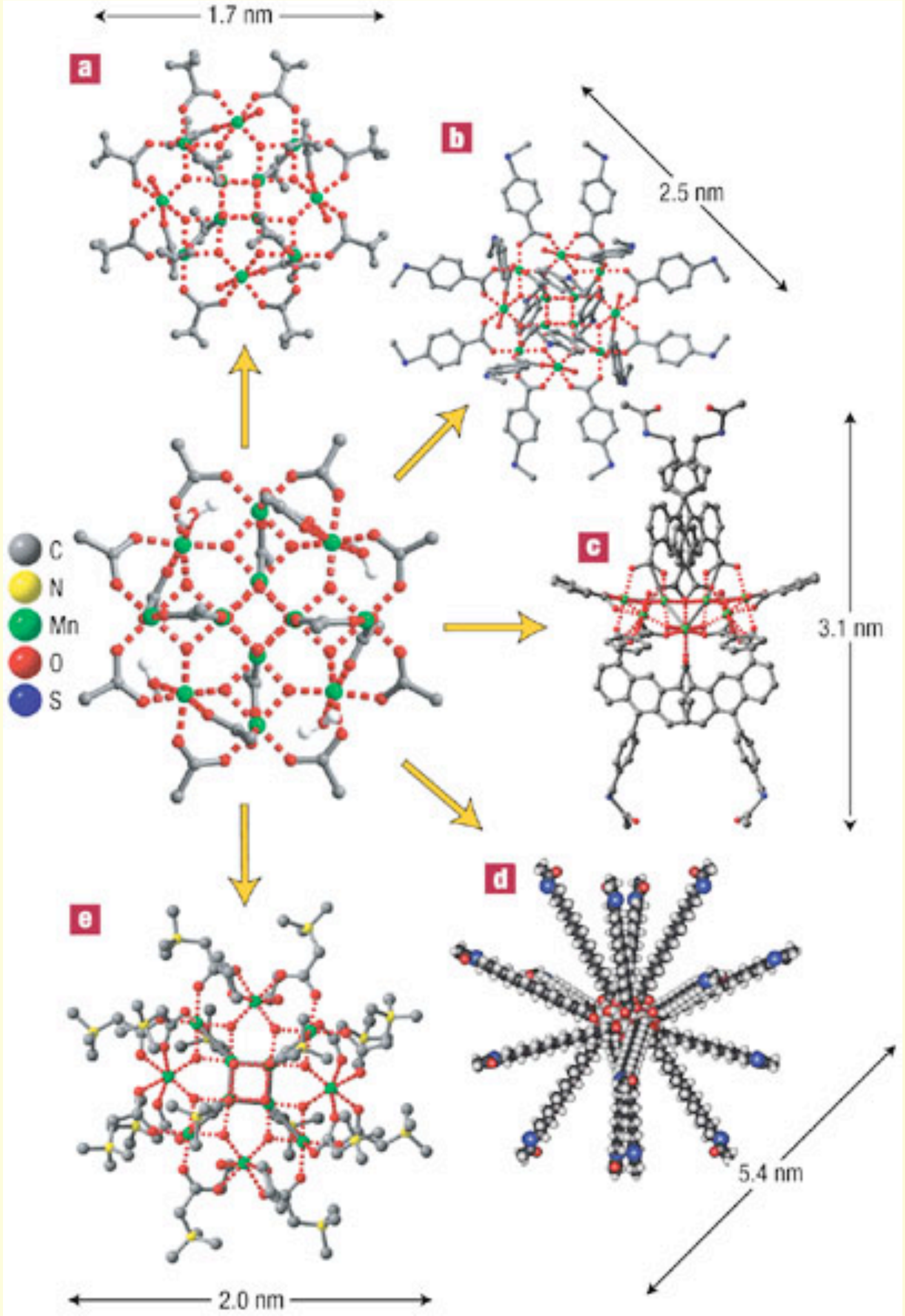


* *Diagram from: Varma, Nature* ***468*** *(2010)*

Magnetism



Magnetostructural transitions
[from Liu *et al.*, Scripta Materialia **66** (2012)]



Single-Molecule Magnets
[from Bogani *et al.*, Nature Materials **7** (2008)]

Formal Construction of FT Density Functionals

Statistical Averages

$$A[\hat{\Gamma}] = \mathrm{Tr}\ \{\hat{\Gamma}\hat{A}\} = \sum_N \sum_i w_{N,i} \langle \Psi_{N,i} | \hat{A} | \Psi_{N,i} \rangle$$

Statistical operator: $\hat{\Gamma} = \sum_{N,i} w_{N,i} |\Psi_{N,i}\rangle\langle\Psi_{N,i}|$

Pure state (orthonormal): $\left\{ |\Psi_{N,i}\rangle \right\}$

Statistical weights (normalized): $\left\{ w_{N,i} \right\}$

Grand Canonical Operator

$$\hat{\Omega} \quad = \quad \hat{H} - \tau\hat{S} - \mu\hat{N}$$

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

Entropy: $\hat{S} = -\ k \ln \hat{\Gamma}$

and $\hat{N}$ *is the particle-number operator.*

At Equilibrium

Variational principle (Gibbs):

$$\Omega^{\tau}_{v-\mu} = \min_{\hat{\Gamma}} \left\{ \Omega[\hat{\Gamma}] \right\}$$

Minimizing Statistical Operator

$$\hat{\Gamma}^0 = \sum_{N,i} w^0_{N,i} |\Psi^0_{N,i}\rangle\langle\Psi^0_{N,i}|$$

At Equilibrium

$$\hat{\Gamma}^0 = \sum_{N,i} w^0_{N,i} |\Psi^0_{N,i}\rangle\langle\Psi^0_{N,i}|$$

where

$$\hat{H}|\Psi^0_{N,i}\rangle = E^0_{N,i}|\Psi^0_{N,i}\rangle$$

$$w^0_{N,i} = \frac{\exp[-\beta(E^0_{N,i}-\mu N)]}{\sum_{N,i}\exp[-\beta(E^0_{N,i}-\mu N)]}$$

$$\beta = \frac{1}{k\tau}$$

Following DF-Fashion

Alternatively:

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

Mermin, Phys. Rev., 137, A1441 (1965)

"Thermal Properties of the Inhomogeneous Electron Gas"

* *See also: Kohn and Sham, Phys. Rev.* ***140*** *(1965)*

At Equilibrium

Variational principle:

$$\Omega^{\tau}_{v-\mu} = \min_{\hat{\Gamma}} \left\{ \Omega[\hat{\Gamma}] \right\}$$

Minimizing Statistical Operator

$$\hat{\Gamma}^0 = \sum_{N,i} w^0_{N,i} |\Psi^0_{N,i}\rangle\langle\Psi^0_{N,i}|$$

Constraint-Search Construction

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

Alternatively:

$$F^{\tau}[n] := \min_{\hat{\Gamma}\to n} \left\{ T[\hat{\Gamma}] + V_{\mathrm{ee}}[\hat{\Gamma}] - \tau S[\hat{\Gamma}] \right\}$$

$$= \min_{\hat{\Gamma}\to n} F^{\tau}[\hat{\Gamma}] = F^{\tau}[\hat{\Gamma}^{\tau}[n]]$$

Constraint-Search Construction

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

Alternatively:

$$\begin{aligned} F^{\tau}[n] &:= \min_{\hat{\Gamma}\to n} \left\{ T[\hat{\Gamma}] + V_{\mathrm{ee}}[\hat{\Gamma}] - \tau S[\hat{\Gamma}] \right\} \\ &= \min_{\hat{\Gamma}\to n} F^{\tau}[\hat{\Gamma}] = F^{\tau}[\hat{\Gamma}^{\tau}[n]] \end{aligned}$$

Constraint-Search Construction

The *non-interacting* analog is

$$
\begin{aligned}
F_{\mathrm{S}}^{\tau}[n] \quad &:= \quad \min_{\hat{\Gamma}\to n} \left\{ T[\hat{\Gamma}] - \tau S[\hat{\Gamma}] \right\} \\
&= \quad \min_{\hat{\Gamma}\to n} K^{\tau}[\hat{\Gamma}] = K^{\tau}[\hat{\Gamma}_{\mathrm{S}}^{\tau}[n]]
\end{aligned}
$$

We refer to $K^{\tau}[\hat{\Gamma}]$ as the "kentropy" to emphasize both the kinetic and entropy contributions.

Kohn-Sham System at FT

Through the KS system, one gets

$$F^\tau[n] = F_{\mathrm{S}}^\tau[n] + U^\tau[n] + \Omega_{\mathrm{X}}^\tau[n] + \Omega_{\mathrm{C}}^\tau[n]$$

where

$$F_{\mathrm{S}}^\tau[n] := K^\tau[\hat{\Gamma}_{\mathrm{S}}^\tau[n]]$$

$$\Omega_{\mathrm{X}}^\tau[n] := V_{ee}[\hat{\Gamma}_{\mathrm{S}}^\tau[n]] - U^\tau[n]$$

$$\Omega_{\mathrm{C}}^\tau[n] := F^\tau[\hat{\Gamma}^\tau[n]] - F^\tau[\hat{\Gamma}_{\mathrm{S}}^\tau[n]] - V_{ee}[\hat{\Gamma}_{\mathrm{S}}^\tau[n]]$$

Kohn-Sham System at FT

Through the KS system, one gets

$$F^{\tau}[n] = F_{\mathrm{S}}^{\tau}[n] + U^{\tau}[n] + \Omega_{\mathrm{X}}^{\tau}[n] + \Omega_{\mathrm{C}}^{\tau}[n]$$

where

$$F_{\mathrm{S}}^{\tau}[n] := K^{\tau}[\hat{\Gamma}_{\mathrm{S}}^{\tau}[n]]$$

$$\Omega_{\mathrm{X}}^{\tau}[n] := V_{ee}[\hat{\Gamma}_{\mathrm{S}}^{\tau}[n]] - U^{\tau}[n]$$

$$\Omega_{\mathrm{C}}^{\tau}[n] := F^{\tau}[\hat{\Gamma}^{\tau}[n]] - F^{\tau}[\hat{\Gamma}_{\mathrm{S}}^{\tau}[n]] - V_{ee}[\hat{\Gamma}_{\mathrm{S}}^{\tau}[n]]$$

Kohn-Sham System at FT

Through the KS system, one gets

$$F^\tau[n] = F_s^\tau[n] + U^\tau[n] + \Omega_x^\tau[n] + \Omega_c^\tau[n]$$

where

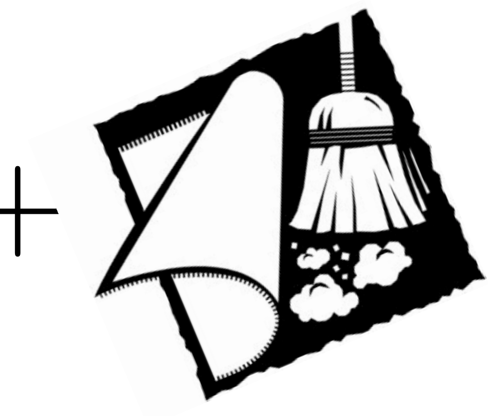
$$F_s^\tau[n] := K^\tau[\hat{\Gamma}_s^\tau[n]]$$

$$\Omega_x^\tau[n] := V_{ee}[\hat{\Gamma}_s^\tau[n]] - U^\tau[n]$$

$$\Omega_c^\tau[n] := F^\tau[\hat{\Gamma}^\tau[n]] - F^\tau[\hat{\Gamma}_s^\tau[n]] - V_{ee}[\hat{\Gamma}_s^\tau[n]]$$

Kohn-Sham System at FT

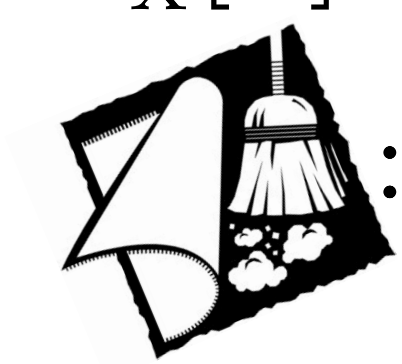
Through the KS system, one gets

$$F^{\tau}[n] = F_{\mathrm{S}}^{\tau}[n] + U^{\tau}[n] + \Omega_{\mathrm{X}}^{\tau}[n] +$$ 

where

$$F_{\mathrm{S}}^{\tau}[n] := K^{\tau}[\hat{\Gamma}_{\mathrm{S}}^{\tau}[n]]$$

$$\Omega_{\mathrm{X}}^{\tau}[n] := V_{ee}[\hat{\Gamma}_{\mathrm{S}}^{\tau}[n]] - U^{\tau}[n]$$

 $$:= F^{\tau}[\hat{\Gamma}^{\tau}[n]] - F^{\tau}[\hat{\Gamma}_{\mathrm{S}}^{\tau}[n]] - V_{ee}[\hat{\Gamma}_{\mathrm{S}}^{\tau}[n]]$$

Under the "Carpet"

$$\Omega_{\mathrm{C}}^{\tau}[n] := E_{\mathrm{C}}^{\tau}[n] - \tau S_{\mathrm{C}}^{\tau}[n] = K_{\mathrm{C}}^{\tau}[n] + U_{\mathrm{C}}^{\tau}[n]$$

where

$$E_{\mathrm{C}}^{\tau}[n] := T_{\mathrm{C}}^{\tau}[n] + U_{\mathrm{C}}^{\tau}[n]$$

$$T_{\mathrm{C}}^{\tau}[n] := T[\hat{\Gamma}^{\tau}[n]] - T[\hat{\Gamma}_{\mathrm{S}}^{\tau}[n]]$$

$$U_{\mathrm{C}}^{\tau}[n] := V_{ee}[\hat{\Gamma}^{\tau}[n]] - V_{ee}[\hat{\Gamma}_{\mathrm{S}}^{\tau}[n]]$$

Under the "Carpet"

$$\Omega_{\mathrm{C}}^{\tau}[n] := E_{\mathrm{C}}^{\tau}[n] - \tau S_{\mathrm{C}}^{\tau}[n] = K_{\mathrm{C}}^{\tau}[n] + U_{\mathrm{C}}^{\tau}[n]$$

where

$$E_{\mathrm{C}}^{\tau}[n] := T_{\mathrm{C}}^{\tau}[n] + U_{\mathrm{C}}^{\tau}[n]$$

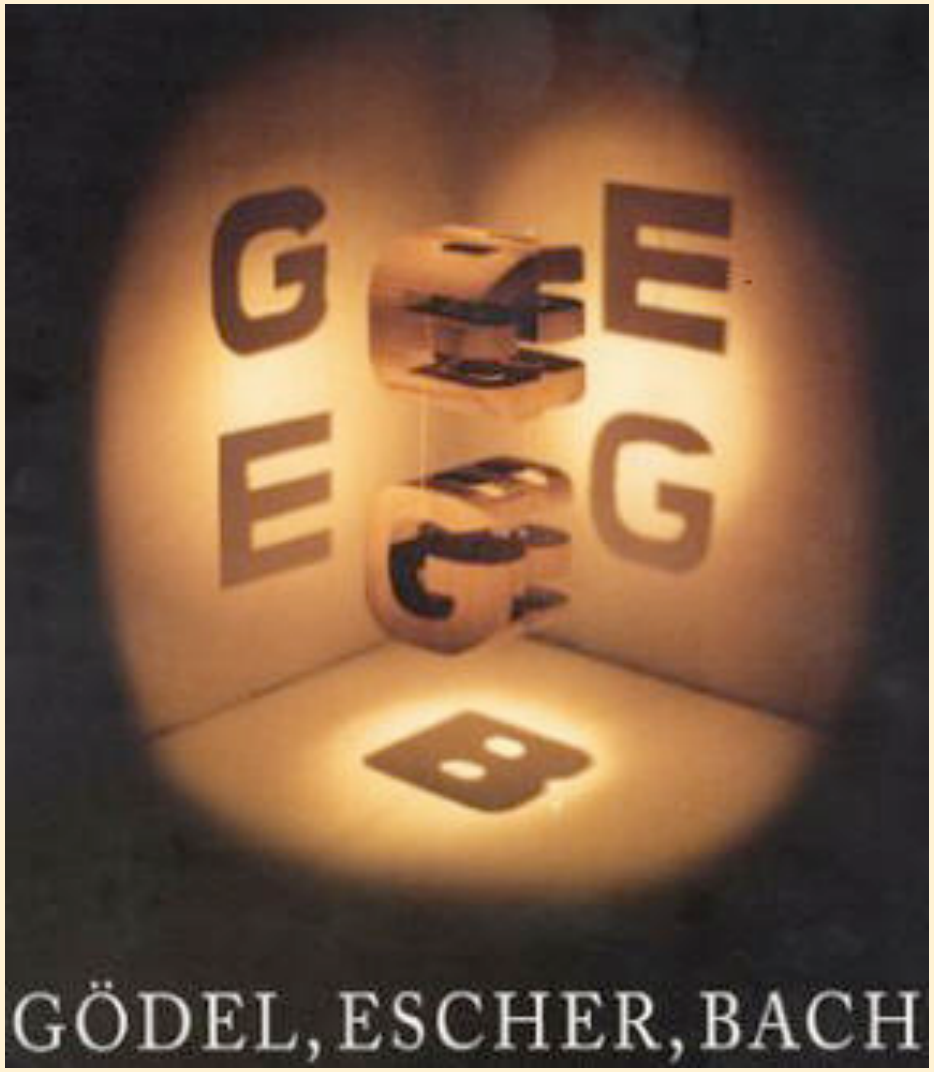
$$T_{\mathrm{C}}^{\tau}[n] := T[\hat{\Gamma}^{\tau}[n]] - T[\hat{\Gamma}_{\mathrm{S}}^{\tau}[n]]$$

$$U_{\mathrm{C}}^{\tau}[n] := V_{ee}[\hat{\Gamma}^{\tau}[n]] - V_{ee}[\hat{\Gamma}_{\mathrm{S}}^{\tau}[n]]$$

$$S_{\mathrm{C}}^{\tau}[n] := S[\hat{\Gamma}^{\tau}[n]] - S[\hat{\Gamma}_{\mathrm{S}}^{\tau}[n]]$$

$$K_{\mathrm{C}}^{\tau}[n] := K[\hat{\Gamma}^{\tau}[n]] - K[\hat{\Gamma}_{\mathrm{S}}^{\tau}[n]]$$

How do they really look?



Cover of the book:
"Gödel, Escher, Bach: An Eternal Golden Braid"
by Douglas Hofstadter (1979)

Some Elementary Facts

Signs of Basic Quantities

Consider

$$K_{\mathrm{C}}^{\tau}[n] := K[\hat{\Gamma}^{\tau}[n]] - K[\hat{\Gamma}_{\mathrm{S}}^{\tau}[n]]$$

Since $\hat{\Gamma}_{\mathrm{S}}^{\tau}[n]$ *minimizes* $K^{\tau}[\hat{\Gamma}]$:

$$K_{\mathrm{C}}^{\tau}[n] \geq 0$$

Signs of Basic Quantities

Consider

$$\Omega_{\mathrm{C}}^{\tau}[n] := F^{\tau}[\hat{\Gamma}^{\tau}[n]] - F^{\tau}[\hat{\Gamma}_{\mathrm{S}}^{\tau}[n]] - V_{ee}[\hat{\Gamma}_{\mathrm{S}}^{\tau}[n]]$$

Since $\hat{\Gamma}^{\tau}[n]$ *minimizes* $F^{\tau}[\hat{\Gamma}]$:

$$\Omega_{\mathrm{C}}^{\tau}[n] \leq 0$$

Signs of Basic Quantities

Since
$$K^{\tau}_{\mathrm{C}}[n] = T^{\tau}_{\mathrm{C}}[n] - \tau S^{\tau}_{\mathrm{C}}[n] \geq 0$$

and
$$\Omega^{\tau}_{\mathrm{C}}[n] = E^{\tau}_{\mathrm{C}}[n] - \tau S^{\tau}_{\mathrm{C}}[n] \leq 0$$

combining with
$$\Omega^{\tau}_{\mathrm{C}}[n] = K^{\tau}_{\mathrm{C}}[n] + U^{\tau}_{\mathrm{C}}[n]$$

gives:
$$U^{\tau}_{\mathrm{C}}[n] \leq 0$$

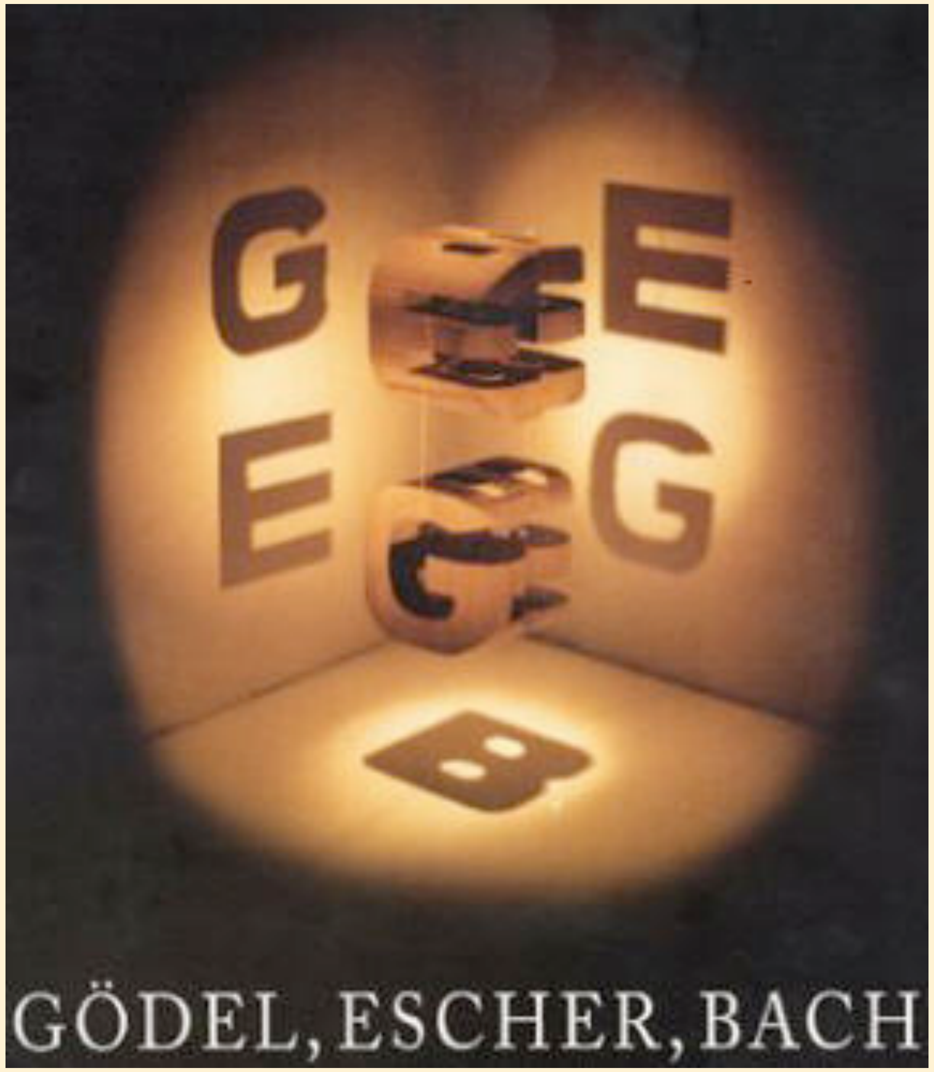
Signs of Basic Quantities

Also, it is true

$$\Omega_{\mathrm{x}}^{\tau}[n] \leq 0$$

** See also: Goerling's lectures in this workshop.*

How do they really look?



Cover of the book:
"Gödel, Escher, Bach: An Eternal Golden Braid"
by Douglas Hofstadter (1979)

Scaling in FT-DFT

Scaling Wavefunctions

Reminder:

$$\Psi^{\gamma}(\mathbf{r}_1, ..., \mathbf{r}_N) := \gamma^{\frac{3}{2}N}\Psi(\gamma\mathbf{r}_1, ..., \gamma\mathbf{r}_N)$$

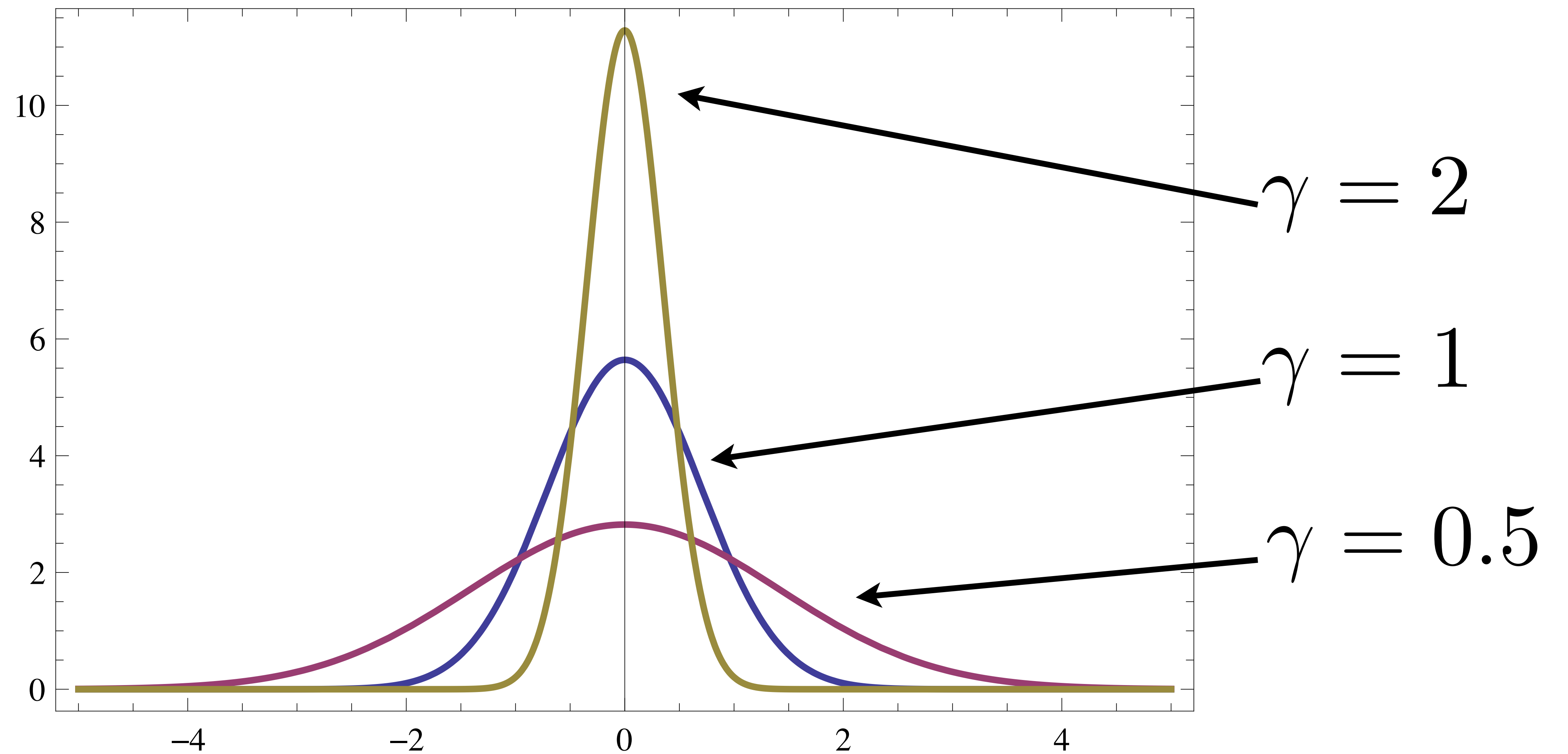
Scale coordinates and keep normalization constant.

M. Levy and J.P. Perdew, Phys. Rev. A **32** (1985)

Scaling Wavefunctions

Correspondingly: $n_\gamma(\mathbf{r}) = \gamma^3 n(\gamma\mathbf{r})$

<u>Example:</u>
N = 10
Dim = 1



M. Levy and J.P. Perdew, Phys. Rev. A **32** (1985)

Scaling Ensembles

We propose

$$\hat{\Gamma}_\gamma := \sum_N \sum_i w_{N,i} |\Psi^\gamma_{N,i}\rangle\langle\Psi^\gamma_{N,i}|$$

Pure states are scaled as usual

$$\Psi^\gamma(\mathbf{r}_1, ..., \mathbf{r}_N) = \langle \mathbf{r}_1, ..., \mathbf{r}_N | \Psi^\gamma \rangle$$

Statistical weight ARE KEPT FIXED!

Scaling of Statistical Averages

Therefore:

$$
\begin{aligned}
T[\hat{\Gamma}_\gamma] &= \gamma^2 T[\hat{\Gamma}] \\
V_{\mathrm{ee}}[\hat{\Gamma}_\gamma] &= \gamma V_{\mathrm{ee}}[\hat{\Gamma}] \\
N[\hat{\Gamma}_\gamma] &= N[\hat{\Gamma}] \\
S[\hat{\Gamma}_\gamma] &= S[\hat{\Gamma}]
\end{aligned}
$$

* *Use Statistical Operators built with orthonormal pure states.*

What happens to the FT Density functionals?

Non-interacting Case

Because

$$K^{\tau}[\hat{\Gamma}_{\gamma}] = \gamma^2 \left(T[\hat{\Gamma}] - \frac{\tau}{\gamma^2} S[\hat{\Gamma}] \right) = \gamma^2 K^{\tau/\gamma^2}[\hat{\Gamma}]$$

We get:

$$\hat{\Gamma}^{\tau}_{\mathrm{S}}[n_{\gamma}] = \hat{\Gamma}^{\tau/\gamma^2}_{\mathrm{S},\gamma}[n]$$

Non-interacting Case

Homogeneous scaling relations:

$$F_{\mathrm{S}}^{\tau}[n_\gamma] = \gamma^2\, F_{\mathrm{S}}^{\tau/\gamma^2}[n]$$
$$S_{\mathrm{S}}^{\tau}[n_\gamma] = S_{\mathrm{S}}^{\tau/\gamma^2}[n]$$

* *See also: Dufty and Trickey, Phys. Rev. B **84** (2011)*

Non-interacting Case

Interesting consequences of

$$F_{\mathrm{S}}^{\tau}[n_\gamma] = \gamma^2\, F_{\mathrm{S}}^{\tau/\gamma^2}[n]$$
$$S_{\mathrm{S}}^{\tau}[n_\gamma] = S_{\mathrm{S}}^{\tau/\gamma^2}[n]$$

High-dens. ~ Low-temp.

$$T_{\mathrm{S}}[n] = \lim_{\gamma\to\infty} F_{\mathrm{S}}^{\tau}[n_\gamma]/\gamma^2$$

Low-dens. ~ High-temp.

$$S_{\mathrm{S}}^{\infty}[n] = -\lim_{\gamma\to 0} F_{\mathrm{S}}^{\tau}[n_\gamma]/\tau$$

Non-interacting Case

Interesting consequences of

$$F_S^\tau[n_\gamma] = \gamma^2\, F_S^{\tau/\gamma^2}[n]$$

Temp-dependence generated through scaling:

$$F_S^{\tau'}[n] = \frac{\tau'}{\tau} F_S^\tau[n_{\sqrt{\tau/\tau'}}]$$

What about the interacting functionals?

Scaling of Statistical Averages

$$\begin{aligned} T[\hat{\Gamma}_\gamma] &= \gamma^2 T[\hat{\Gamma}] \\ V_{\rm ee}[\hat{\Gamma}_\gamma] &= \gamma V_{\rm ee}[\hat{\Gamma}] \\ N[\hat{\Gamma}_\gamma] &= N[\hat{\Gamma}] \\ S[\hat{\Gamma}_\gamma] &= S[\hat{\Gamma}] \end{aligned}$$

** Use Statistical Operators built with orthonormal pure states.*

Interacting Case

Since:

$$K^{\tau}[\hat{\Gamma}_{\lambda}] + \lambda V_{ee}[\hat{\Gamma}_{\lambda}] = \lambda^2 \left\{ K^{\tau/\lambda^2}[\hat{\Gamma}] + V_{ee}[\hat{\Gamma}] \right\}$$

and

$$F^{\tau,\lambda}[n] = \min_{\hat{\Gamma}\to n} \left\{ T[\hat{\Gamma}] + \lambda\, V_{\mathrm{ee}}[\hat{\Gamma}] - \tau S[\hat{\Gamma}] \right\}$$

We get:

$$\hat{\Gamma}^{\tau,\lambda}[n_{\lambda}] = \hat{\Gamma}_{\lambda}^{\tau/\lambda^2}[n]$$

Interacting Case

Homogeneous scaling relations:

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

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

* *See also: lecture given by Dufty in March meeting APS (2012)*

Homogeneous Scaling

Interesting consequence of

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

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

High-dens. ~ Low-temp.

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

Low-dens. ~ High-temp.

$$S^\infty[n] = -\lim_{\lambda\to 0} F^{\tau,\lambda}[n_\lambda]/\tau$$

Homogeneous Scaling

Interesting consequence of

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

Temp-dependence generated through scaling:

$$F^{\tau'}[n] = \frac{\tau'}{\tau} F^{\tau,\sqrt{\tau/\tau'}}[n_{\sqrt{\tau/\tau'}}]$$

For Fixed Coupling

What if…

we don't scale the strength of the interaction?

For Fixed Coupling

Inequality!

$$K^{\tau}[n_\gamma] + V_{\rm ee}^{\tau}[n_\gamma] \leq \gamma^2\, K^{\tau/\gamma^2}[n] + \gamma\, V_{\rm ee}^{\tau/\gamma^2}[n]$$

this is because:

$$\Gamma^{\tau}[n_\gamma] \neq \Gamma_\gamma^{\tau/\gamma^2}[n]$$

Lots of Inequalities!

For $\lambda = 1$ and $\gamma \geq 1$

$$
\begin{aligned}
K^{\tau}[n_\gamma] &\leq \gamma^2\, K^{\tau/\gamma^2}[n] \\
V_{\mathrm{ee}}^{\tau}[n_\gamma] &\geq \gamma\, V_{\mathrm{ee}}^{\tau/\gamma^2}[n] \\
K_{\mathrm{C}}^{\tau}[n_\gamma] &\leq \gamma^2\, K_{\mathrm{C}}^{\tau/\gamma^2}[n] \\
U_{\mathrm{C}}^{\tau}[n_\gamma] &\geq \gamma\, U_{\mathrm{C}}^{\tau/\gamma^2}[n] \\
\Omega_{\mathrm{C}}^{\tau}[n_\gamma] &\geq \gamma\, \Omega_{\mathrm{C}}^{\tau/\gamma^2}[n]
\end{aligned}
$$

Exchange

Homogeneous scaling relation

$$\Omega_{\mathrm{x}}^{\tau}[n_\gamma] = \gamma\, \Omega_{\mathrm{x}}^{\tau/\gamma^2}[n]$$

EXX and GGAs

Homogeneous scaling relation:

$$\Omega_{\mathrm{X}}^{\tau}[n_\gamma] = \gamma\,\Omega_{\mathrm{X}}^{\tau/\gamma^2}[n]$$

Constraint for FT-GGA construction

$$\omega_{\mathrm{X}}^{\mathrm{GGA}\tau}(n(\mathbf{r}), |\nabla n|(\mathbf{r})) = e_{\mathrm{X}}^{\mathrm{unif}}(n(\mathbf{r}))\, F_{\mathrm{X}}(s(\mathbf{r}), \tilde{\tau}(\mathbf{r}))$$

$$\tilde{\tau}(\mathbf{r}) \approx \tau/n^{2/3}(\mathbf{r})$$

$$s \approx |\nabla n|/(n^{4/3})$$

* *See also: poster presented by Karasiev in this workshop.*

XC from Coupling Integration

Coupling constant integration

$$\Omega^{\tau}_{\mathrm{XC}}[n] = \int_0^1 d\lambda\, V^{\tau,\lambda}_{ee}[n] - U^{\tau}[n]$$

We can avoid in this way to deal with the correlation "Kentropy".

X from XC

$$\Omega_{\mathrm{x}}^{\tau}[n] = \lim_{\gamma\to\infty} \Omega_{\mathrm{xc}}^{\gamma^2\tau}[n_\gamma]/\gamma$$

This is useful to define/extract the "exchange" part of a given XC approximation.

Conclusions and Outlooks

Phys. Rev. Lett., 107, 163001 (2011)

Derived several exact properties
of Finite-Temperature DFT functionals
useful for constraining approximations.

What's next?

(a) Derivation of *new approximations*;
(b) APPLICATIONS.

Acknowledgments

DFG, DOE, NSF

- Dr. A. Floris
  King's College, London, U.K.
- Dr. A. Sanna
  Max-Planck Institute, Halle, Germany
- Dr. C. Bersier
  Max-Planck Institute, Halle, Germany
- Prof. C. Proetto
  Centro Atomico Bariloche, Argentina
- Prof. K. Burke
  University of California, Irvine
- Prof. E.K.U. Gross
  Max-Planck Institute, Halle, Germany

THANK YOU

FOR YOUR ATTENTION!