Fundamentals of Density Functional Theory & Selected progress in \textit{ab initio} nuclear DFT

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December 22, 2017
Fundamentals of Density Functional Theory

- Interesting viewpoints on DFT
- Hohenberg-Kohn (HK) theorem
- Kohn-Sham (KS) scheme
- Discussions and open issues

Selected progress in *ab initio* nuclear DFT

- Relativistic Brueckner-Hartree-Fock (RBHF) theory
- *A bridge*: inverse Kohn-Sham (iKS) method
- Functional Renormalization Group (FRG)
- *Application*: $\phi^4$-theory in zero dimension
“Although QCD is the basic theory of strong interactions, other models must take over for a proper description of the low-energy nuclear behavior.”

“The figure indicates some models used and their region of applicability.”

“Note that the regions overlap, we are progressing towards a complete understanding of nuclear structure.”

Proper energy scale & degree of freedom for understanding the proper physics
Nuclear many-body problem

Nuclear $N$-particle system

- Time-dependent Schrödinger/Dirac equation (in this talk $\hbar = c = 1$)
  \[ i \frac{\partial \Psi(t)}{\partial t} = \hat{H} \Psi(t) \]

- Stationary equation
  \[ \hat{H} \Psi(x_1, x_2, \ldots, x_N) = E \Psi(x_1, x_2, \ldots, x_N) \]
  where $x_i = (r_i, \sigma_i, \tau_i)$ stands for the spatial, spin, and isospin coordinates.

  The problem becomes extremely difficult when $N = 4, 5, 6, \ldots$

- However, the $N$-particle wave function contains a great deal of information, which is irrelevant to most of important physical properties.

- It is very advantageous to introduce the density matrices, defined from the many-body wave function by integrating out much of redundant information.
One-body local density

(a function in 3D space, independent of $N$)

$$\rho(r) = \sum_{\sigma, \tau} \int |\Psi(x_1, x_2, \ldots, x_N)|^2 dx_2 \ldots dx_N$$

- experimental observable
- with transparent physical meaning
- easily visualized

The aim of density functional theory (DFT) is

- to reduce the many-body quantum mechanical problem formulated in terms of $N$-particle wave functions $\Psi$ to the one-particle level with the local density distribution $\rho(r)$.

http://www.nishina.riken.go.jp/index_e.html
State-of-the-art nuclear theories

Density functional theory (DFT) aims at understanding both ground-state and excited-state properties of thousands of nuclei in a consistent and predictive way.
Impacts of DFT

Nobel Prize 1998
"for his development of the density-functional theory"

Number of annual citations of HK1964 & KS1965 data from Web of Science

4000
58,000 +

- “A work of fundamental importance is usually much quoted directly after is publication, but no longer so when it has entered textbooks and has become canonized. Why did this not happen to the Hohenberg-Kohn paper?”

- “Actually the HK theorem is a rather unusual kind of theorem, that resists an easy interpretation, and that has still a touch of mystery.”

—— Werner Kutzelnigg
Nobel Lecture: Electronic structure of matter—wave functions and density functionals

W. Kohn

Department of Physics, University of California, Santa Barbara, California 93106

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Density functional theory in terms of a Legendre transformation for beginners

Werner Kutzelnigg *

Lehrstuhl für Theoretische Chemie, Ruhr-Universität Bochum, D-44780 Bochum, Germany

Received 3 May 2006; accepted 3 May 2006
Available online 22 May 2006

Abstract

The derivation of the Hohenberg–Kohn (HK) theorem by means of a simplified version of Lieb’s Legendre transformation is presented, with the stress on physically problematic aspects, and caring about the definition of the domains of the respective functionals only to the extent, that this is absolutely necessary. The take-home lesson consists in a critical analysis of some statements often found in the DFT literature. As a simple illustration for a Legendre transformation we discuss that in parameter space for the family of $n$-electron isoelectronic atomic ions, with the nuclear charge as parameter.

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HK original paper [Phys. Rev. 136, B864 (1964)]

- We develop an **exact formal variational principle** for the ground-state energy $E$, in which the density $\rho(r)$ is the variable function.
- Into this principle enters a **universal functional** $F_{HK}[\rho(r)]$, which applies to all electronic systems in their ground state no matter what the external potential $u(r)$ is.
- The main objective of theoretical considerations is a description of this functional. **Once known**, it is relatively easy to determine the ground-state energy in a given external potential.

**Basic lemma of HK** [Nobel Lecture]

- The ground-state density $\rho(r)$ of a bound system of interacting electrons in some external potential $u(r)$ determines this potential **uniquely**.
In proving their theorem, Hohenberg and Kohn considered a collection of an arbitrary number of electrons enclosed in a large box, moving under the influence of an external potential $u(r)$ and the mutual Coulomb repulsion.

- Hamiltonian with an external field
  \[ \hat{H}_u = \hat{T} + \hat{V}_{cc} + \hat{U} \quad \text{with} \quad \hat{U} = \int dx \psi^\dagger(x) u(r) \psi(x) \]

- Schrödinger equation
  \[ \hat{H}_u \Psi_u(x_1, x_2, \ldots, x_N) = E_u \Psi_u(x_1, x_2, \ldots, x_N) \]

- One-body local density
  \[ \rho(r) = \sum_{\sigma, \tau} \int |\Psi(x, x_2, \ldots, x_N)|^2 dx_2 \ldots dx_N \]

- Obviously, $\Psi_u$ and $\rho(r)$ are uniquely determined by $u(r)$.

To prove $u(r)$ is uniquely determined by $\rho(r)$

Proof of Hohenberg-Kohn theorem (II)

- Assume that another potential \( u'(\mathbf{r}) \) leads to the ground-state wave function \( \Psi_{u'} \), and the energy \( E_{u'} \), but gives rise to the same density \( \rho'(\mathbf{r}) = \rho(\mathbf{r}) \).

- According to Rayleigh-Ritz minimal principle

\[
E_{u'} = \langle \Psi_{u'} | \hat{H}_{u'} | \Psi_{u'} \rangle < \langle \Psi_u | \hat{H}_u | \Psi_u \rangle = E_u + \langle \Psi_u | \hat{U}' - \hat{U} | \Psi_u \rangle
\]

i.e.,

\[
E_{u'} < E_u + \int d\mathbf{r} [u'(\mathbf{r}) - u(\mathbf{r})] \rho(\mathbf{r})
\]

- Exactly, in the same way, one gets

\[
E_u < E_{u'} + \int d\mathbf{r} [u(\mathbf{r}) - u'(\mathbf{r})] \rho(\mathbf{r})
\]

\[
E_u + E_{u'} < E_u + E_{u'}
\]

\[
\rho'(\mathbf{r}) \neq \rho(\mathbf{r})
\]

- Therefore, \( u(\mathbf{r}) \) is uniquely determined by \( \rho(\mathbf{r}) \), so are Hamiltonian \( H_u \), wave function \( \Psi_u \), and the expectation values of all operators of interest.
In general, one can obtain the ground-state energy $E_u$ of $H_u$ by

$$E_u = \min_{\tilde{\Psi}} \langle \tilde{\Psi} | \hat{T} + \hat{V}_{cc} + \hat{U} | \tilde{\Psi} \rangle$$

Two-step constrained search method

1. Fix a trial ground-state density $\tilde{\rho}(\mathbf{r})$, denoting $\tilde{\Psi}_{\tilde{\rho}}$ the class of trial wave functions with this density

$$E_u[\tilde{\rho}(\mathbf{r})] = \min_{\tilde{\Psi}_{\tilde{\rho}}} \langle \tilde{\Psi}_{\tilde{\rho}} | \hat{T} + \hat{V}_{cc} + \hat{U} | \tilde{\Psi}_{\tilde{\rho}} \rangle = F_{\text{HK}}[\tilde{\rho}(\mathbf{r})] + \int u(\mathbf{r})\tilde{\rho}(\mathbf{r})d\mathbf{r}$$

where

$$F_{\text{HK}}[\tilde{\rho}(\mathbf{r})] = \min_{\tilde{\Psi}_{\tilde{\rho}}} \langle \tilde{\Psi}_{\tilde{\rho}} | \hat{T} + \hat{V}_{cc} | \tilde{\Psi}_{\tilde{\rho}} \rangle$$

2. Minimize $E_u$ over all $\tilde{\rho}(\mathbf{r})$

$$E_u = \min_{\tilde{\rho}} \left\{ F_{\text{HK}}[\tilde{\rho}(\mathbf{r})] + \int u(\mathbf{r})\tilde{\rho}(\mathbf{r})d\mathbf{r} \right\}$$

- $F_{\text{HK}}[\rho(\mathbf{r})]$ requires no explicit knowledge of $u(\mathbf{r})$.
- It is a universal functional of the density $\rho(\mathbf{r})$. 
HK variational principle (III)

- **HK variation principle**

\[
\delta E_u = \int \text{d}r \left\{ \frac{\delta F_{\text{HK}}}{\delta \tilde{\rho}(\mathbf{r})} + u(\mathbf{r}) - \mu \right\} \delta \tilde{\rho}(\mathbf{r}) = 0
\]

- **Euler-Lagrange equations**

\[
\left\{ \frac{\delta F_{\text{HK}}}{\delta \tilde{\rho}(\mathbf{r})} + u(\mathbf{r}) - \mu \right\} \delta \tilde{\rho}(\mathbf{r}) = 0
\]

with Lagrange multiplier \( \mu \), chemical potential.
**Exercise: Non-interacting system**

\[
F_{\text{HK}}[\hat{\rho}(\mathbf{r})] \Rightarrow T_0[\hat{\rho}(\mathbf{r})] = \min_{\hat{\Psi}} \langle \hat{\Psi} \hat{\rho} | \hat{T} | \hat{\Psi} \hat{\rho} \rangle
\]

\[
\left\{ \frac{\delta T_0}{\delta \hat{\rho}^{\ast}(\mathbf{r})} + u(\mathbf{r}) - \mu \right\} \delta \hat{\rho}(\mathbf{r}) = 0
\]

- However, even in this simple case, the functional \( T_0[\rho(\mathbf{r})] \) is unknown.

**We are in the fortunate situation that**

- One-body local density \( \rho(\mathbf{r}) = \sum_{i=1}^{N} \varphi_i^{\ast}(\mathbf{r}) \varphi_i(\mathbf{r}) \)

- Expectation value of kinetic energy \( T_0 = \langle \hat{T} \rangle = \sum_{i=1}^{N} \langle \varphi_i | - \frac{1}{2M} \nabla^2 | \varphi_i \rangle \)

- Thus

\[
\frac{\delta T_0}{\delta \varphi_i^{\ast}(\mathbf{r})} = -\frac{1}{2M} \nabla^2 \varphi_i(\mathbf{r})
\]

\[
\frac{\delta T_0}{\delta \varphi_i^{\ast}(\mathbf{r})} = \int d\mathbf{r}' \frac{\delta T_0}{\delta \rho(\mathbf{r}')} \frac{\delta \rho(\mathbf{r}')}{\delta \varphi_i^{\ast}(\mathbf{r})} = \frac{\delta T_0}{\delta \rho(\mathbf{r})} \varphi_i(\mathbf{r})
\]
If we get the solutions of Schrödinger equation exactly

\[ \left\{ \frac{1}{2M} \nabla^2 + u(r) - \epsilon_i \right\} \varphi_i(r) = 0 \]

we get the solution of the HK variation principle.

\[ \left\{ \frac{\delta T_0}{\delta \rho(r)} + u(r) - \mu \right\} \delta \rho(r) = 0 \]

“*We are so in the curious situation, that we are able to solve the HK variational equations, without even knowing anything about the functional $F_{HK}$, nor its derivative (except that they exist).”*

“**DFT without a density functional**”

The unknown functional $F_{HK}[\rho(r)]$ is decomposed into two parts

$$F_{HK}[\tilde{\rho}(r)] = T_0[\tilde{\rho}(r)] + I[\tilde{\rho}(r)]$$

- $I[\rho(r)] = \text{interaction energy} + (T - T_0)$ ← $T$ the actual kinetic energy

To solve Euler-Lagrange equations for HK variation principle

$$\left\{ \frac{\delta T_0}{\delta \tilde{\rho}(r)} + u_{KS}(r) - \mu \right\} \delta \tilde{\rho}(r) = 0 \quad \text{where} \quad u_{KS}(r) = u(r) + \frac{\delta I}{\delta \tilde{\rho}(r)}$$

by solving KS equations (self-consistently)

$$\left\{ -\frac{1}{2M} \nabla^2 + u_{KS}(r) - \epsilon_i \right\} \varphi_i(r) = 0$$

always local?
Once $F_{HK}$ is known ...

- Once the universal functional $F_{HK}[\rho(r)]$ is known, it is relatively easy to determine the ground-state energy in a given external potential.

\[
E_u = \min_{\tilde{\rho}} \left\{ F_{HK}[\tilde{\rho}(r)] + \int u(r)\tilde{\rho}(r)dr \right\}
\]

- Note that

$F_{HK}[\tilde{\rho}(r)] = \min_{\tilde{\Psi}} \langle \tilde{\Psi}|\hat{T} + \hat{V}_{ee}|\tilde{\Psi}\rangle$ as complicated as $E_u = \min_{\tilde{\Psi}} \langle \tilde{\Psi}|\hat{T} + \hat{V}_{ee} + \hat{U}|\tilde{\Psi}\rangle$

- Alternatively,

$F_{HK}[\tilde{\rho}(r)] = \sup_{\tilde{u}} \left\{ E[\tilde{u}(r)] - \int \tilde{u}(r)\tilde{\rho}(r)dr \right\}$

This is not a very realistic assumption.

- Why should we assume that the more difficult problem to know $E(u)$ for a family of $u$ is solved, if we are interested in the much simpler problem to obtain $E(u)$ for a single $u$?

The Fundamentals of Density Functional Theory (revised and extended version)

H. Eschrig

$$y = f(x)$$

$$y = f(x_0)x - f^*$$

$$f^*(p) = \sup_x \{ px - f(x) \}$$

$$p = \frac{df}{dx}$$

From wikipedia

5 Legendre Transformation
5.1 Elementary Introduction
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5.3 Prelude on Lebesgue Integral
5.4 Banach Space
5.5 Dual Space
5.6 Conjugate Functionals
5.7 The Functional Derivative
5.8 Lagrange Multipliers

6 Density Functional Theory by Lieb
6.1 The Ground State Energy
6.2 The Hohenberg-Kohn Variational Principle
6.3 The Functionals $F$, $G$, and $H$
6.4 The Kohn-Sham Equation

Keys
Convex-functional analysis
Legendre transformation
Mathematical foundations of DFT

Functionals

- $E[u(r)], F_{HK}[\rho(r)]$ ✓ vs $\Psi[u(r)], \Psi[\rho(r)]$ ✗
- Functionals have well-defined domains and analytic properties, that, e.g., allow the construction of Legendre transformations.

From $E[u(r)]$ to $F_{HK}[\rho(r)]$
- $E[u(r)]$ is a concave functional in $u \in L^{3/2} + L^{\infty}$
- Legendre transformation is well defined
  $$F_{HK}[\tilde{\rho}(r)] = \sup_{\tilde{u}} \left\{ E[\tilde{u}(r)] - \int \tilde{u}(r)\tilde{\rho}(r)dr \right\}$$

From $F_{HK}[\rho(r)]$ to $E[u(r)]$
- $F_{HK}[\rho(r)]$ is a convex functional in $\rho \in L^{3} \cap L^{1}$
- Legendre transformation is well defined
  $$E[u(r)] = \inf_{\tilde{\rho}} \left\{ F_{HK}[\tilde{\rho}(r)] + \int u(r)\tilde{\rho}(r)dr \right\}$$

Nucleus is a self-bound system (without external potential)

- It is somewhat useless to use the ground-state density in the laboratory frame, because $\rho(r) = N/V \rightarrow 0$ ($V \rightarrow \infty$).
- DFT theorem for the intrinsic density $\rho_{\text{intr.}}(r)$ (a wave-packet state)

$$ |\Psi\rangle = |\Phi\rangle \otimes |\chi\rangle $$

where $\Phi$ indicates the intrinsic state and $\chi$ defines the spurious motion.

See, e.g., Review

RECOMMENDATIONS OF MODERN PHYSICS, VOLUME 88, OCTOBER–DECEMBER 2016

Time-dependent density-functional description of nuclear dynamics

Nakatsukasa, Matsuyanagi, Matsuo, Yabana, RMP 88, 045004 (2016)

Open questions:

- What is the domain of $\rho_{\text{intr.}}(r)$?
- Is $F[\rho_{\text{intr.}}(r)]$ strictly convex in this domain?
Nucleus is a self-bound system (without external potential)

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See, e.g., Review Nakatsukasa, Matsuyanagi, Matsuo, Yabana, RMP 88, 045004 (2016)

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Zhou, Phys. Scr. 91, 063008 (2016)
Fundamentals of Density Functional Theory
- Interesting viewpoints on DFT
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- Kohn-Sham (KS) scheme
- Discussions and open issues

Selected progress in ab initio nuclear DFT
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Covariant density functional theory (CDFT)

- **Fundamental:** Kohn-Sham Density Functional Theory
- **Scheme:** Yukawa meson-exchange nuclear interactions

\[
\mathcal{L} = \bar{\psi} \left[ i \gamma^\mu \partial_\mu - M - g_\sigma \sigma - \gamma^\mu \left( g_\omega \omega_\mu + g_\rho \vec{\rho} \cdot \vec{\rho}_\mu + \frac{1}{2} \gamma^3 A_\mu \right) - \frac{f_\pi}{m_\pi} \gamma_5 \gamma^\mu \partial_\mu \vec{\pi} \cdot \vec{\tau} \right] \psi \\
+ \frac{1}{2} \partial^\mu \sigma \partial_\mu \sigma - \frac{1}{2} m_\sigma^2 \sigma^2 - \frac{1}{4} \Omega^{\mu\nu} \Omega_{\mu\nu} + \frac{1}{2} m_\omega^2 \omega_\mu \omega^\mu - \frac{1}{4} \vec{R} \cdot \vec{R}_{\mu\nu} + \frac{1}{2} m_\rho^2 \vec{\rho}_\mu \cdot \vec{\rho}_\mu \\
+ \frac{1}{2} \partial_\mu \vec{\pi} \cdot \partial^\mu \vec{\pi} - \frac{1}{2} m_\pi^2 \vec{\pi} \cdot \vec{\pi} - \frac{1}{4} F_{\mu\nu} F^{\mu\nu}
\]

Comparing to traditional non-relativistic DFT

- **Effective Lagrangian**
  connections to underlying theories, QCD at low energy
- **Dirac equation**
  consistent treatment of spin d.o.f. & nuclear saturation properties (3-body effect)
- **Lorentz covariant symmetry**
  unification of time-even and time-odd components


cf. Meng’s talk

Nobel Prize 1949
Nobel Prize 1998
Tensor effects in CDFT?

Tensor effects are crucial, in particular, for properties of exotic nuclei

\[ j_z \quad (a) \quad j_z' \quad (b) \]

\[ j_z \quad j_z' \quad \text{attraction} \]
\[ j_z \quad j_z' \quad \text{repulsion} \]

\[ \text{proton} \quad \text{neutron} \]

\[ \text{π meson (tensor) is not welcomed in CDFT} \]

\[ \text{new magic numbers} \]


What are the tensor effects in CDFT?


Ab initio for CDFT

some fingerprints

N = 82
**Ab initio for CDFT**

- Brueckner-Hartree-Fock theory (*ladder diagrams to all order*)
  - cf. Sibo Wang and Hui Tong’s talks
  - (with exchange terms as well)

\[
\begin{align*}
\text{HF} & \quad d \\
\begin{array}{c}
c \\
\end{array} & +
\begin{array}{c}
c \\
\end{array} \\
\end{align*}
\]

\[
\begin{align*}
\text{BHF} & \\
\begin{array}{c}
c \\
\end{array} & d \\
\end{align*}
\]

- Bethe-Goldstone equation $\rightarrow$ **finite nuclei**

\[
\langle ab | G(W) | cd \rangle = \langle ab | V | cd \rangle + \sum_{mn} \langle ab | V | mn \rangle \frac{Q(m, n)}{W - \varepsilon_m - \varepsilon_n} \langle mn | G(W) | cd \rangle
\]

where the starting energy $W = \varepsilon_c + \varepsilon_d$

For the first time, **Bethe-Goldstone equation** is solved **self-consistently**

- in the **rest** frame
- in pure **relativistic** scheme

PKU scholarship & RIKEN IPA project

Relativistic BHF calculations for $^{16}$O with Bonn A interaction

- A first *ab initio* calculations for finite nuclei in relativistic scheme
- Spin-orbit splitting is reproduced well from the bare interaction
- Benchmark for various LDA calculations

EDA = effective density approximation [Müther(1990)]
LDA = local density approximation

Neutron drops

Neutron drop is a multi-neutron system confined in an external field.

Why neutron drops?

- simple, can be accessed by many ab initio methods
- an ideal environment for studying neutron rich system

Pudliner et al., *PRL* 76, 2416 (1996)
Maris et al., *PRC* 87, 054318 (2013)
Potter et al., *PLB* 739, 445 (2014)
Zhao & Gandolfi, *PRC* 94, 041302(R) (2016)

- Relativistic Hartree-Fock (RHF) equation with external field

\[ (T + U + U_{ex}) |a\rangle = e_a |a\rangle, \quad U_{ij} = \sum_{c=1}^{A} \langle ic | \tilde{G}(W) | jc \rangle \]
Object: neutron drops with neutron number \( N \) from 4 to 50

External field: **spherical harmonic oscillator** (HO) potential

\[
U_{ex} = \frac{1}{2} M \omega^2 r^2 \quad \text{with} \quad \hbar \omega = 10 \text{ MeV}
\]

Interaction: Bonn A

Cut-offs for basis space: \( l_{cut} = 24, \varepsilon_{cut} = 1000 \text{ MeV}, \varepsilon_{Dcut} = -1700 \text{ MeV} \)

Total angular momentum cut-off \( J_{cut} = 12 \)

Basis: self-consistent RHF basis

Box size: \( R = 8 \text{ fm} \)
Energies and radii

- Relativistic BHF calculations for neutron drops with Bonn A interaction

- Energies $E$ and radii $R_N$ are consistent with JISP16 or AV8’.

- $R_N$ follows the $N^{1/6}$ law.

Shen, HZL, Meng, Ring, Zhang, arXiv:1709.06289

Maris et al., *PRC* 87, 054318 (2013)
Potter et al., *PLB* 739, 445 (2014)
Spin-orbit splitting (RBHF)

The SO splitting decreases as the spin-up $j_>= l + 1/2$ orbitals are filled, while the SO splitting increases as the spin-down $j_< = l + 1/2$ orbitals are filled.


Tensor effect in relativistic scheme

Shen, HZL, Meng, Ring, Zhang, arXiv:1709.06289
Spin-orbit splitting (RMF)

Comparison with the **phenomenological** relativistic mean-field (RMF) energy density functionals (EDF).

None of them can reproduce this tensor behavior!
Spin-orbit splitting (RHF)

- Comparison with the **phenomenological** relativistic Hartree-Fock (RHF) energy density functionals (EDF).

- RHF (PKO1) shows a very similar pattern, mainly contributed by $\pi_{NN}$ tensor interaction.

- Neither RBHF nor CDFT includes beyond-mean-field effects → it is a fair comparison!

Then what?

Shen, HZL, Meng, Ring, Zhang, arXiv:1709.06289
A bridge between ab initio and DFT

**CDFT:** RMF or RHF

\[
L = \bar{\psi} \left[ i \gamma^\mu \partial_\mu - M - g_\sigma \sigma - \gamma^\mu \left( g_\omega \omega_\mu + g_\rho \vec{\tau} \cdot \vec{\rho}_\mu + e \frac{1 - \tau_3}{2} A_\mu \right) - \frac{f_\pi}{m_\pi} \gamma^5 \gamma^\nu \partial_\mu \vec{\tau} \cdot \vec{\tau} \psi \right] \\
+ \frac{1}{2} \partial^\mu \sigma \partial_\mu \sigma - \frac{1}{2} m_\sigma^2 \sigma^2 - \frac{1}{4} \Omega^\mu\nu \Omega_{\mu\nu} + \frac{1}{2} m_\omega^2 \omega_\mu \omega^\mu - \frac{1}{4} \overline{R}_{\mu\nu} \cdot \overline{R}^{\mu\nu} + \frac{1}{2} m_\rho^2 \rho^\mu \cdot \rho_\mu \\
+ \frac{1}{2} \partial_\mu \vec{\nu} \cdot \partial^\nu \vec{\nu} - \frac{1}{2} m_\pi^2 \vec{\nu} \cdot \vec{\nu} - \frac{1}{4} F^{\mu\nu} F_{\mu\nu}
\]


**Construction of exact Kohn-Sham orbitals from a given electron density**

Yue Wang and Robert G. Parr  
*Department of Chemistry, University of North Carolina, Chapel Hill, North Carolina 27599*  
(Received 27 May 1992)

This paper prescribes an orbital construction of the exact local effective potential in the Kohn-Sham self-consistent equations, so that from a given electron density the corresponding exact Kohn-Sham potential and orbitals may be found self-consistently. It also shows the convergence of the method if the system is \( \nu \) representable.

**A possible strategy?**

- **Inputs:** all possible kinds of densities from ab initio calculations / exp. data
- **Outputs:** a systematic way to write down new terms in EDF
Fundamentals of Density Functional Theory

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A dream for next-generation DFT

quantum-field-theory oriented DFT

EDF from effective action

\[ F_{HK}[\rho] \sim \Gamma[\rho]/\beta \]

(Legendre transform)

non-perturbative nature by renormalization group

\[ \partial_k \Gamma_k[\rho] = \text{Tr}\{\ldots\} \]

(flow eq.)

theoretical uncertainties from EFT

\( \Gamma^{(2)}, \Gamma^{(3)}, \Gamma^{(4)} \ldots \)

(power counting)

Interdisciplinary:
(lattice) QCD

hadron

cold atom

condensed matter

quantum chemistry

……

also cf.


Kutzelnigg, JMS 768, 163 (2006)

Drut, Furnstahl, Platter, PPNP 64, 120 (2010)

Braun, JPG 39, 033001 (2012)

Metzner et al., RMP 84, 299 (2012)

Drews & Weise, PPNP 93, 69 (2017)

……
The aim of density functional theory (DFT) is

- to reduce the many-body quantum mechanical problem formulated in terms of \( N \)-particle wave functions \( \Psi \) to the one-particle level with the local density distribution \( \rho(x) \).

**Hohenberg-Kohn theorem** [Phys. Rev. 136, B864 (1964)]

- There exist a **universal density functional** \( F_{HK}[\rho(x)] \).
- The ground-state energy \( E_{gs} \) attains its minimum value when the density \( \rho(x) \) has its correct ground-state value.

**HK variational principle**

\[
E_U = \inf_{\rho} \left\{ F_{HK}[\rho(x)] + \int d^d x \, U(x) \rho(x) \right\}
\]

Where \( F_{HK}[\rho(x)] = \min_{\Psi} \langle \Psi | \hat{T} + \hat{V} | \Psi \rangle \) is a **universal functional**, which is valid for any number of particles \( N \) and for any external field \( U(x) \).
EDF from effective action

Strategy: $F_{\text{HK}}[\rho] \leftrightarrow \Gamma[\rho] \leftrightarrow \text{partition function} \leftrightarrow \text{path integral}$

- Classical action in Euclidean space
  
  \[ S_E[\psi^\dagger, \psi] = \int_0^\beta d\tau \int d^d x \psi^\dagger(\tau, x) \left( \frac{\partial}{\partial \tau} - \frac{\nabla^2}{2M} + U(x) \right) \psi(\tau, x) \]
  
  \[ + \frac{1}{2} \int_0^\beta d\tau \int d^d x_1 d^d x_2 \psi^\dagger(\tau, x_1) \psi^\dagger(\tau, x_2) V(x_1, x_2) \psi(\tau, x_2) \psi(\tau, x_1) \]

  where $U(x)$ is one-body potential and $V(x_1, x_2)$ is two-body interaction.

- Partition function in two-particle point-irreducible ($2\text{PPI}$) scheme

  \[ Z[J] = \int \mathcal{D}\psi^\dagger \mathcal{D}\psi \exp \left[ -S[\psi^\dagger, \psi] + \int_0^\beta d\tau \int d^d x J(\tau, x) \psi^\dagger(\tau, x) \psi(\tau, x) \right] \]

  external source $J$ couples $\psi^\dagger \psi$ at the same space-time.

- Thermodynamic potential / generating function / Schwinger function

  \[ W[J] = \ln Z[J] \]

  \[ E_{\text{gs}} = \lim_{\beta \to \infty} -\frac{1}{\beta} W \]
Connection to Hohenberg-Kohn theorem

- Local density
  \[ \rho(\tau, x) = \langle \psi^\dagger(\tau, x)\psi(\tau, x) \rangle = \frac{\delta W[J]}{\delta J(\tau, x)} \]

- Effective action \( \xrightarrow{\text{Legendre transform}} \) of \( W \) with respect to \( J \)
  \[ \Gamma[\rho] = \sup_{\{J\}} \left\{ -W[J] + \int_0^\beta d\tau \int d^dx \, J(\tau, x)\rho(\tau, x) \right\} \]

- The universality of the Hohenberg-Kohn functional \( F_{HK}[\rho] \) follows from the fact that the background \( U \) potential can be absorbed into the source terms \( J \) by a simple shift \( J \rightarrow J - U \).

Second Legendre transform \( \rightarrow \) HK variation

\[ E_U = \inf_{\rho} \left\{ F_{HK}[\rho(x)] + \int d^d x \, U(x)\rho(x) \right\} \]
Non-perturbative nature of interaction

- Lippmann-Schwinger eq. / Bethe-Goldstone eq. / Brueckner theory
  Brueckner Hartree-Fock, hole-line expansion … (in 1960s, 70s)

Relativistic BHF for finite nuclei
Shen, Hu, HZL, Meng, Ring, Zhang,
Shen, HZL, Meng, Ring, Zhang,


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**Exact evolution equation for the effective potential**

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**Flow equation**

\[
\frac{\partial}{\partial k} \Gamma_k[\phi] = \frac{1}{2} \text{Tr} \left\{ \left[ \Gamma_k^{(2)}[\phi] + R_k \right]^{-1} \frac{\partial}{\partial k} R_k \right\} = \frac{1}{2} \]

*Cited 1500+ times* (google scholar, November 2017)

in QCD, hadron, nuclear, cold atom, condensed matter, quantum chemistry ……
Non-perturbative nature of interaction

- Lippmann-Schwinger eq. / Bethe-Goldstone eq. / Brueckner theory
  Brueckner Hartree-Fock, hole-line expansion … (in 1960s, 70s)

Relativistic BHF for finite nuclei
Shen, Hu, HZL, Meng, Ring, Zhang,
Shen, HZL, Meng, Ring, Zhang,
PRC 96, 014316 (2017)

- Functional Renormalization Group (FRG) --- Wetterich, PLB 301, 90 (1993)


Flow equation
\[
\partial_\lambda \Gamma_\lambda[\rho] = \text{Tr} \left\{ (\partial_\lambda U_\lambda) \cdot \rho + \frac{1}{2} \rho \cdot V \cdot \rho + \frac{1}{2} V \cdot \left[ \Gamma_\lambda^{(2)} \right]^{-1} \right\}
\]
Theoretical uncertainty

- **FRG Flow equation**: a set of coupled differential equations (infinite hierarchy)

- Proper power counting by $\Gamma^{(0)}, \Gamma^{(2)}, \Gamma^{(3)}, \Gamma^{(4)} \ldots$?

- Controllable theoretical uncertainty?
φ⁴-theory in zero dimension

Model setup

- Classical action (0D in space-time, bosonic d.o.f.)
  \[ S[\varphi] = \frac{1}{2} \omega^2 \varphi^2 + \frac{1}{24} v \varphi^4 \]

- Partition function (2PPI scheme)
  \[ Z[J] = \int_{-\infty}^{\infty} d\varphi \exp\{-S[\varphi] + J \varphi^2\} \]

Exact solution

- Ground-state energy (\(v_0 = v/\omega^4\))
  \[ E_{gs} = Z[0]/Z_0 = \int_{-\infty}^{\infty} d\varphi \exp\{-S[\varphi]\}/Z_0 = \sqrt{\frac{3}{2\pi v_0}} K_1^{1/4} \left( \frac{3}{4v_0} \right) e^{3v_0} \]

- Ground-state density
  \[ \rho_{gs} = \langle \varphi^2 \rangle = \frac{1}{Z} \frac{\delta Z[J]}{\delta J} \bigg|_{J=0} \]
  \[ = \frac{1}{\omega^2} \left[ \frac{3}{2} K_5^{1/4} \left( \frac{3}{4v_0} \right) + \frac{3}{2} K_{-3/4} \left( \frac{3}{4v_0} \right) - (v_0 + 3) K_1^{1/4} \left( \frac{3}{4v_0} \right) \right] / \left[ v_0 K_1^{1/4} \left( \frac{3}{4v_0} \right) \right] \]
Typical cases

$v/\omega^4 = 0.01$

$v/\omega^4 = 1$

$v/\omega^4 = 100$

perturbative   non-perturbative   highly non-perturbative

$\rho_{gs} = \omega^{-2} \left( 1 - \frac{v_0}{2} + \frac{2v_0^2}{3} - \frac{11v_0^3}{8} + \frac{34v_0^4}{9} + \ldots \right)$

$E_{gs} = \frac{v_0}{8} - \frac{v_0^2}{12} + \frac{11v_0^3}{96} - \frac{17v_0^4}{72} + \ldots$

Keitel & Bartosch, JPA 45, 105401 (2012)
Kemler & Braun, JPG 40, 085105 (2013)
FRG for 0D $\phi^4$-theory

- **FRG + DFT Flow equation**

$$\partial_\lambda \Gamma_\lambda[\rho] = \text{Tr} \left\{ (\partial_\lambda U_\lambda) \cdot \rho + \frac{1}{2} \rho \cdot V \cdot \rho + \frac{1}{2} V \cdot \left[ \Gamma_\lambda^{(2)} \right]^{-1} \right\}$$

$$\partial_\lambda \Gamma_\lambda[\rho] = \frac{1}{24} v \left[ \rho^2 + \left( \Gamma_\lambda^{(2)}[\rho] \right)^{-1} \right]$$

- **Conventional expansion** Kemler & Braun, *JPG* 40, 085105 (2013)

$$\Gamma_\lambda[\rho] = \Gamma_\lambda^{(0)}[\bar{\rho}_\lambda] + \sum_{n=2}^{\infty} \frac{1}{n!} \Gamma_\lambda^{(n)}[\bar{\rho}_\lambda] (\rho - \bar{\rho}_\lambda)^n$$

- **Coupled differential equations**

$$\partial_\lambda \Gamma_\lambda^{(0)}[\rho_\lambda] = \frac{1}{24} v \left[ \rho_\lambda^2 + G_\lambda[\rho_\lambda] \right]$$

$$\partial_\lambda \rho_\lambda = -\frac{1}{24} v \left[ 2 \rho_\lambda G_\lambda[\rho_\lambda] - \Gamma_\lambda^{(3)}[\rho_\lambda] G_\lambda^3[\rho_\lambda] \right]$$

$$\partial_\lambda \Gamma_\lambda^{(2)}[\rho_\lambda] = \frac{1}{24} v \left[ 2 + 3(\Gamma_\lambda^{(3)})^2 G_\lambda^3 - 2 \rho_\lambda \Gamma_\lambda^{(3)} G_\lambda \right] \rho_\lambda$$

$$\partial_\lambda \Gamma_\lambda^{(3)}[\rho_\lambda] = -\frac{1}{4} v \left[ (\Gamma_\lambda^{(3)})^3 G_\lambda^4 \right] \rho_\lambda$$

...  

...
FRG for 0D $\phi^4$-theory

- **FRG + DFT Flow equation**

$$
\partial_\lambda \Gamma_\lambda[\rho] = \text{Tr} \left\{ (\partial_\lambda U_\lambda) \cdot \rho + \frac{1}{2} \rho \cdot V \cdot \rho + \frac{1}{2} V \cdot \left[ \Gamma_\lambda^{(2)} \right]^{-1} \right\}
$$

$$
\partial_\lambda \Gamma_\lambda[\rho] = \frac{1}{24} v \left[ \rho^2 + \left( \Gamma_\lambda^{(2)}[\rho] \right)^{-1} \right]
$$


$$
\Gamma_\lambda[\rho] = \Gamma_\lambda^{(0)}[\bar{\rho}_\lambda] + \sum_{n=2}^{\infty} \frac{1}{n!} \Gamma_\lambda^{(n)}[\bar{\rho}_\lambda](\rho - \bar{\rho}_\lambda)^n
$$

- Kohn-Sham scheme? uncertainties?

- Up to 6th-order calculation, results are not satisfactory.
Our Ideas

- FRG + DFT Flow equation

\[
\partial_\lambda \Gamma_\lambda[\rho] = \text{Tr} \left\{ (\partial_\lambda U_\lambda) \cdot \rho + \frac{1}{2} \rho \cdot V \cdot \rho + \frac{1}{2} V \cdot \Gamma_\lambda^{(2)} \right\}^{-1}
\]

\[
\partial_\lambda \Gamma_\lambda[\rho] = \frac{1}{24} v \left[ \rho^2 + \left( \Gamma_\lambda^{(2)}[\rho] \right)^{-1} \right]
\]

- Optimized expansion

\[
\Gamma_\lambda[\rho] = \Gamma_{\text{KS},\lambda}[\rho] + \gamma_\lambda[\rho]
\]

  - Non-interacting part

\[
\Gamma_{\text{KS},\lambda}[\rho] = -\frac{1}{2} \ln(\omega^2 \rho) - \frac{1}{2} + \frac{\rho}{2 \bar{\rho}_\lambda}
\]

  - Correlation part

\[
\gamma_\lambda[\rho] = \gamma_\lambda^{(0)}[\bar{\rho}_\lambda] + \sum_{n=2}^{\infty} \frac{1}{n!} \gamma_\lambda^{(n)}[\bar{\rho}_\lambda] (\rho - \bar{\rho}_\lambda)^n
\]

**Ideas of Kohn-Sham**

- To introduce an artificial **non-interacting** system which provides the same ground-state density \(\rho_{\text{gs}}\) with a **Kohn-Sham** (mean-field) potential

- **Difference** between interacting and non-interacting systems is absorbed in the correlation (**beyond-mean-field**) part of EDF, \(E_x[\rho]\).
Optimized FRG + DFT

- Coupled differential equations

\[
\begin{align*}
\partial_\lambda \rho_\lambda &= -\frac{1}{24} v \left[ 2\rho G_\lambda + \left( \frac{1}{\rho^3} - \gamma_\lambda^{(3)} \right) G_\lambda^3 \right] \bar{\rho}_\lambda \\
\partial_\lambda \gamma_\lambda^{(0)}[\rho_\lambda] &= \frac{1}{24} v \left[ \rho^2 - \frac{1}{2\rho} \left( \frac{1}{\rho^3} - \gamma_\lambda^{(3)} \right) G_\lambda^3 \right] \bar{\rho}_\lambda \\
\partial_\lambda \gamma_\lambda^{(2)}[\rho_\lambda] &= \frac{1}{24} v \left[ 2 - 2\rho \gamma_\lambda^{(3)} G_\lambda - \left( \frac{3}{\rho^4} + \gamma_\lambda^{(4)} \right) G_\lambda^2 + \left( \frac{1}{\rho^3} - \gamma_\lambda^{(3)} \right) \left( \frac{2}{\rho^3} - 3\gamma_\lambda^{(3)} \right) G_\lambda^3 \right] \bar{\rho}_\lambda \\
\partial_\lambda \gamma_\lambda^{(3)}[\rho_\lambda] &= \frac{1}{24} v \left[ -2\rho \gamma_\lambda^{(4)} G_\lambda + \frac{12}{\rho^5} G_\lambda^2 - \left( \frac{1}{\rho^3} - \gamma_\lambda^{(3)} \right) \left( \frac{18}{\rho^4} + 7\gamma_\lambda^{(4)} \right) G_\lambda^3 + 6 \left( \frac{1}{\rho^3} - \gamma_\lambda^{(3)} \right)^3 G_\lambda^4 \right] \bar{\rho}_\lambda \\
\partial_\lambda \gamma_\lambda^{(4)}[\rho_\lambda] &= \frac{1}{24} v \left[ -\frac{60}{\rho^6} G_\lambda^2 + \frac{96}{\rho^5} \left( \frac{1}{\rho^3} - \gamma_\lambda^{(3)} \right) G_\lambda^3 + 6 \left( \frac{3}{\rho^4} + \gamma_\lambda^{(4)} \right)^2 G_\lambda^3 \\
&\quad - 36 \left( \frac{1}{\rho^3} - \gamma_\lambda^{(3)} \right)^2 \left( \frac{3}{\rho^4} + \gamma_\lambda^{(4)} \right) G_\lambda^4 + 24 \left( \frac{1}{\rho^3} - \gamma_\lambda^{(3)} \right)^4 G_\lambda^5 \right] \bar{\rho}_\lambda 
\end{align*}
\]

To solve

- Estimating upper/lower bounds

- Keeping as KS counterparts
Typical cases (I)

- Perturbative case $v_0 = v/\omega^4 = 0.01$

- Effective action vs density, $F_{HK}[\rho]$.

- 1st-order optimized FRG result is on top of the exact solution in a very large density region.

- Theoretical uncertainty is invisible in the figure.
Typical cases (III)

- Non-perturbative case \( v_0 = v/\omega^4 = 1 \)

- 1st-order result reproduces the exact solution in a wide density region, with corresponding uncertainty.

- 2nd-order result does improve.

- Effective action vs density, \( F_{HK}[\rho] \).

KS optimized FRG

Kemler & Braun (2013)
Typical cases (III)

- Highly non-perturbative case $v_0 = \frac{v}{\omega^4} = 100$

- 1st-order result is still able to describe the exact solution with large uncertainty.

- 2nd-order and 3rd-order results improve step by step
  — accuracy of $\rho_{gs}$ increases by factor 4, $E_{gs}$ by factor 10 at each order.
In summary

- **Ground-state densities and energies:** $\phi^4$-theory in 0D

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<td>$E_{gs}$</td>
<td>$\rho_{gs}$</td>
<td>$E_{gs}$</td>
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<td>$0.001241785^{+55}_{-19}$</td>
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<td>2nd-order</td>
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<td>3rd-order</td>
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<tr>
<td>exact</td>
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</table>

**DFT ↔ ideas of QFT (effective action + RG + EFT)**

- EDF $F_{HK}[\rho]$ is derived from effective action $\Gamma[\rho]$ in 2PPI scheme with Legendre transform.
- Non-perturbative nature of interaction is handled by FRG with flow equation.
- Beyond-mean-field effects $\gamma^{(n)}$ in $F_{HK}[\rho]$ are taken into account order-by-order with (proper) theoretical uncertainties.

from $\phi^4$-theory in 0D to 3+1D finite nuclei …
Further reading

A shortest cut for understanding DFT


Recent reviews


Toward future developments