Toward Ab Initio DFT for Nuclei: The Optimized Effective Potential

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Plan

- Two roads to ab initio DFT
  - Density Matrix Expansion
  - Optimized Effective Potential
    - Three comments
    - Solving the OEP equation exactly

- OEP for Pairing

- Done & to do
Two roads to ab initio DFT

**Road 1** Density Matrix Expansion (DME)  (Negele & Vautherin)

- Expand the **density matrix (DM)** in terms of **local densities**, **gradients**, and **kinetic energy densities**.

\[
\rho(R_1, R_2)
\]

**Angle averaged DM**

\[
\hat{\rho}(R + s/2, R - s/2)
\]
Two roads to ab initio DFT

**Road 1**
Density Matrix Expansion (DME)  (Negele & Vautherin)

- Expand the density matrix (DM) in terms of local densities, gradients, and kinetic energy densities.

\[
\hat{\rho}(R + s/2, R - s/2) = \frac{1}{2} \int dx \exp \left[ x \cdot s \cdot (\nabla_1 - \nabla_2)/2 \right] \rho(R_1, R_2) \bigg|_{R_1 = R_2 = R} \\
= \frac{1}{sk_F(R)} \left[ \sum_{n=0}^{\infty} (4n + 3)j_{2n+1}(sk_F(R)) Q_n \left( \frac{(\nabla_1 - \nabla_2)^2}{2k_F(R)} \right) \right] \rho(R_1, R_2) \bigg|_{R_1 = R_2 = R} \\
\approx \rho_{SL}(k_F(R)s) \rho(R) + s^2 g(k_F(R)s) \left[ \frac{1}{4} \nabla^2 \rho(R) - \tau(R) + \frac{3}{5} k_F(R)^2 \rho(R) \right]
\]

\( k_F \) is an arbitrary scale (here \( k_F(R) = (3\pi^2 \rho(R)/2)^{1/3} \)) of no effect if all terms are included.

- See talk by J. Dobaczewski

- Phase-space averaging techniques improve on plain DME dramatically! (DME-PSA, see talk by Scott Bogner)

Tuesday, June 22, 2010
Two roads to ab initio DFT

And he [Jacob] dreamed, and behold a ladder set up on the earth, and the top of it reached to heaven . . . ” [Genesis 28:12]
Two roads to ab initio DFT

- LDA
  “Take the density-dependent energy of the uniform system and replace $\rho$ with $\rho(r)$ ...”
  - Very easy to implement
  - Not very accurate, in many cases not even qualitatively accurate
Two roads to ab initio DFT

- **GGA**  “Take the LDA and add gradient corrections…”
  - Great improvement over LDA
  - Still has some difficult problems: - Absence of negative ions
    - van der Waals forces
    - Self-interaction errors

- **LDA**  “Take the density-dependent energy of the uniform system and replace $\rho$ with $\rho(\mathbf{r})$ …”
  - Very easy to implement
  - Not very accurate, in many cases not even qualitatively
Two roads to ab initio DFT

Optimized Effective Potential (OEP)

“Allow for explicit KS orbital dependence …”
- Harder to implement
- Computationally more expensive
- Allows for exact exchange, solves many of the problems of GGAs

GGA “Take the LDA and add gradient corrections…”
- Great improvement over LDA
- Still has some difficult problems:
  - Absence of negative ions
  - van der Waals forces
  - Self-interaction errors

LDA “Take the density-dependent energy of the uniform system and replace $\rho$ with $\rho(\mathbf{r})$ …”
- Very easy to implement
- Not very accurate, in many cases not even qualitatively
Three comments on the OEP

I. Self-interaction errors  (see Kümmel & Kronik, RMP (2008))

- Each electron feels the repulsion of the total charge of the system, **including its own**!

  Insufficient binding

  Wrong prediction of unstable anions

- Should we worry about this for nuclei?
Three comments on the OEP

II. Derivative discontinuities in \( \mu \equiv \frac{\delta E_{\text{tot}}}{\delta n(r)} \),
(see Kümmel & Kronik, RMP (2008))

Consider two well-separated neutral atoms in equilibrium
i.e. the energy is at a minimum...

Assume \( \mu(X) > \mu(Y) \)

Then we can continuously shift charge from \( Y \) to \( X \) and lower
the energy... but how can the energy be at a new
minimum if the atoms are now charged?!

Paradox. The chemical potential is not a continuous
function of the particle number.

Jacob’s ladder

Tuesday, June 22, 2010
Three comments on the OEP

III. RPA! (Capture low-amplitude collective modes)

- Use adiabatic connection:

\[
E_{xc} = \frac{1}{2} \int d^3r \int d^3r' \frac{e^2}{|\vec{r} - \vec{r}'|} \int_0^1 d\lambda \left( -\frac{1}{\pi} \int_0^\infty d\omega \text{Im} \chi_\lambda(\vec{r}, \vec{r}', \omega) - n(\vec{r}) \delta(\vec{r} - \vec{r}') \right)
\]

\[
\chi_\lambda(\vec{r}, \vec{r}', \omega) = \chi_{KS}(\vec{r}, \vec{r}', \omega) + \int d^3x \int d^3y \chi_{KS}(\vec{r}, \vec{x}, \omega) \left( \frac{\lambda e^2}{|\vec{x} - \vec{y}|} + f_{xc,\lambda}(\vec{x}, \vec{y}, \omega) \right) \chi_\lambda(\vec{y}, \vec{r}', \omega)
\]

\[
\chi_{KS}(\vec{r}, \vec{r}', \omega) = \lim_{\eta \to 0} \sum_{\eta=\uparrow, \downarrow} \sum_{j,k} (f_{k,\sigma} - f_{j,\sigma}) \frac{\varphi_{j,\sigma}(\vec{r}) \varphi_{k,\sigma}^*(\vec{r}) \varphi_{j,\sigma}(\vec{r}') \varphi_{k,\sigma}^*(\vec{r}')}{\omega - (\epsilon_{j,\sigma} - \epsilon_{k,\sigma}) + i\eta}
\]

- Combine with short- and long-range splitting:

\[
\frac{1}{|\vec{r}_i - \vec{r}_j|} = \text{erf}(\mu|\vec{r}_i - \vec{r}_j|) + \frac{1 - \text{erf}(\mu|\vec{r}_i - \vec{r}_j|)}{|\vec{r}_i - \vec{r}_j|}
\]

Jacob’s ladder
Kohn-Sham DFT

- Kohn-Sham approach
  “The density functional can be optimized by solving a Schrödinger-like problem...”

\[
F_{HK}[\rho] = T_s[\rho] + E_{int}[\rho]
\]

- Kohn-Sham equations

\[
\left[ -\frac{\nabla^2}{2m} + v_{KS}(r) \right] \varphi_k(r) = \epsilon_k \varphi_k(r)
\]

- Solve recursively:
  - Start with guess for orbitals
  - Compute potential
  - Solve for orbitals
  
\[
\rho(x) = \sum_{k=1}^{N} |\varphi_k(x)|
\]
The OEP equation

- **OEP integral equation**

\[
\int dx' \ Q(x, x') v_{xc}(x') = \Lambda(x)
\]

\[
Q(x, x') = \sum_{j=1}^{N} \phi_j^*(x') G_j(x', x) \phi_j(x) + \text{c.c.}
\]

\[
\Lambda(x) = \sum_{j=1}^{N} \int dx' \ \phi_j^*(x') u_{xc,j}(x') G_j(x', x) \phi_j(x) + \text{c.c.}
\]

**Green’s function**

\[
G_j(x', x) = \sum_{k \neq j} \frac{\phi_k(x') \phi_k^*(x)}{\epsilon_j - \epsilon_k}
\]

**Auxiliary potential**

\[
u_{xc,j}(x') = \frac{1}{\phi_j^*(x')} \frac{\delta E_{int}}{\delta \phi_j(x')}
\]

- Sum over occupied and unoccupied states!
The OEP equation

- OEP integral equation

\[ \int dx' \, Q(x, x')v_{xc}(x') = \Lambda(x) \]
Solving the OEP equation

Two problems:

- Constructing the Green’s function explicitly may be expensive
- The OEP equation is singular

\[
\sum_{k=1}^{N} \psi_k^*(x) \varphi_k(x) + \text{c.c.} = 0
\]

\[
(\hat{h}_{KS} - \varepsilon_i) \psi_i^*(x) = - \left[ \Delta_i(x) - \bar{\Delta}_i \right] \varphi_i(x)
\]

\[
\Delta_i(x) = v_{xc}(x) - u_{xc,i}(x)
\]

\[
u_{xc,j}(x') = \frac{1}{\varphi_j^*(x')} \frac{\delta E_{int}}{\delta \varphi_j(x')}
\]
Solving the OEP equation

- Kümmel-Perdew Iterative solution
  - Guess xc potential and compute $\psi_i^*(x)$
    \[
    \Delta_i(x) = v_{xc}(x) - u_{xc,i}(x)
    \]
    \[
    (\hat{h}_{KS} - \varepsilon_i)\psi_i^*(x) = - \left[ \Delta_i(x) - \bar{\Delta}_i \right] \varphi_i(x)
    \]
  - Update xc potential
    \[
    v_{xc}^{new} = v_{xc}^{old} + cS(x)
    \]
    \[
    S(x) = \sum_{i=1}^{N} \psi_i^*(x)\varphi_i(x) + c.c.
    \]
  - Recompute $\psi_i^*(x)$
  - Repeat until
    \[
    \sum_{k=1}^{N} \psi_k^*(x)\varphi_k(x) + c.c. = 0
    \]
  - Go back to KS equation and recompute $\varphi_i(x)$

Use Conjugate gradients!
Results in 1D

- Gaussian interaction. Exact exchange functional

8+8 fermions in 1D
Results in 1D

- Gaussian interaction. Exact exchange functional

Density profile
Results in 1D

- Gaussian interaction. Exact exchange functional

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Results in 1D

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- Gaussian interaction. Exact exchange functional

Density profile
Results in 1D

- Gaussian interaction. Exact exchange functional

Density profile
Results in 1D

- Gaussian interaction. Exact exchange functional
- 8 fermions in 1D

Harmonic trap

Negele interaction (2 gaussians)
Results in 1D

- Gaussian interaction. Exact exchange functional

8 fermions in 1D
Results in 1D

• Gaussian interaction. Exact exchange functional

8 fermions in 1D
OEP for pairing

Notation

KS-HFB Equations

\[ h\Phi_k = E_k \Phi_k \]

\[ h_{rr'} = \begin{pmatrix} \hat{h}_s \delta(r-r') & D_s(r,r') \\ D_s^*(r,r') & -\hat{h}_s \delta(r-r') \end{pmatrix} \]

Kohn-Sham potentials

\[ v_s(r) = v_{ext}(r) + v_H(r) + v_{xc}(r) \]

\[ D_s(r,r') = D_{ext}(r,r') + D_H(r,r') + D_{xc}(r,r') \]

Orbitals

\[ \Phi_k(r) = \begin{pmatrix} u_k(r) \\ v_k(r) \end{pmatrix} \]

Exchange-correlation potentials

\[ v_{xc}(r) = \frac{\delta E_{xc}}{\delta n(r)} \]

\[ D_{xc}(r) = -\frac{\delta E_{xc}}{\delta \Delta^*(r,r')} \]

Order parameter fields

\[ n(r) \equiv 2 \sum_k \left[ |u_k(r)|^2 f(E_k) + |v_k(r)|^2 f(-E_k) \right] \]

\[ \Delta(r,r') \equiv \sum_k \left[ v_k^*(r')u_k(r)f(-E_k) + v_k^*(r)u_k(r')f(E_k) \right] \]
OEP for pairing

Two coupled integral equations.

\[ \sum_k \Psi^*_{G,k}(r) \Phi_k(r) = 0 \]

\[ \Psi^*_{G,k}(r) \equiv \int d^3r' G_k(r', r) \left[ \frac{\delta E_{xc}}{\delta \Phi_k(r')} - \int d^3r'' v_{xc}(r'') \frac{\delta n(r'')}{\delta \Phi_k(r')} \right. \]

\[ \left. - \int d^3r'' d^3r''' D_{xc}(r''', r'') \frac{\delta \Delta(r''', r'')}{\delta \Phi_k(r')} \right] \]

\[ \sum_k \Psi^*_{F,k}(r, r') \Phi_k(r) \Phi_k(r') = 0 \]

\[ \Psi^*_{F,k}(r, s) \equiv \int d^3r' F_k(r', r, s) \left[ \frac{\delta E_{xc}}{\delta \Phi_k(r')} - \int d^3r'' v_{xc}(r'') \frac{\delta n(r'')}{\delta \Phi_k(r')} \right. \]

\[ \left. - \int d^3r'' d^3r''' D_{xc}(r''', r'') \frac{\delta \Delta(r''', r'')}{\delta \Phi_k(r')} \right] \]

\[ \frac{\delta \Phi_k(r)}{\delta v_s(r')} = G_k(r, r') \Phi_k(r') \]

\[ \frac{\delta \Phi_k(r)}{\delta D_s(r', r'')} = F_k(r, r', r'') \Phi_k(r') \Phi_k(r''). \]
Done / To do

- Implemented full **OEP** solution in 1D (Kümmel-Perdew algorithm) ✔
  - Allows for orbital-dependent functionals
  - Solves formal and practical problems of GGAs
  - Allows for exact exchange, RPA, Pairing, etc...

- Tested 1D proof-of-concept against Hartree-Fock ✔

- Derived OEP-HFB equations (first time) ✔

- 3D code under development (framework in place, now debugging)

- Minnesota potential & compare with HF, HF-DME, NCSM, GFMC

- RPA?

- QRPA?