

Update on Orbital-based DFT for Nuclei

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UNEDF Collaboration meeting,
East Lansing, MI
Summer solstice 2011.



UNEDF SciDAC Collaboration
Universal Nuclear Energy Density Functional



Colleagues

Dick Furnstahl

The Ohio State University



Lucas Platter

Chalmers University of Technology



More recently...

Created collaborative google site
“OEP in Nuclear Physics” (still private)

The screenshot shows a Google Sites interface for a site titled "OEP in Nuclear Physics". At the top, there are navigation links for Gmail, Calendar, Documents, Photos, Reader, and Web, along with a "more" dropdown. The user's name, "Joaquín E. Drut", and a settings gear icon are in the top right. Below the navigation, the site title "OEP in Nuclear Physics" is displayed in a large, bold font. To the right of the title is a search box with the text "Search this site". Below the title, there is a sidebar on the left with a list of links: "Welcome!", "Codes", "Meetings & Conference calls", "Members", "Our papers", "Plan*" (highlighted in blue), "Useful notes", "Useful references", and "Sitemap". Below the sidebar is a link to "Edit sidebar". The main content area is titled "Plan*" and contains a quote: "*Always under construction. 'Plans are nothing; planning is everything' D. D. Eisenhower." Below the quote is a "Contents" box with two links: "1 Introduction" and "2 Codes". The main content area also has a section titled "Introduction" with a paragraph of text: "The OEP is a method that extends conventional GGA approaches to DFT by allowing for explicit KS orbital dependence in the energy density functionals (EDFs). The prototypical example of an orbital-dependent EDF is the so-called 'exact exchange' functional, which is simply the Hartree-Fock (HF) energy where the HF orbitals are replaced by the KS orbitals. Thus, the OEP enables a direct connection between microscopic interactions (e.g. Coulomb) and EDFs, providing an avenue for *ab initio* DFT. More complex expressions for the energy, such as those derived from perturbation theory beyond HF, are also within the realm of OEP-DFT. It should be noted that this approach has been actively investigated in quantum chemistry, particularly in the last decade, and is currently regarded as the state-of-the-art in that field." Below the introduction is another paragraph: "The benefits of the OEP come at the price of increased formal sophistication and computational demand. Indeed, the OEP method requires the solution of an integral equation (the OEP equation) in order to determine".

More recently...

Created collaborative google site
“OEP in Nuclear Physics” (still private)

Drawing more people into the OEP game
to tackle the various aspects of ab initio
orbital-based nuclear DFT.

Done / To-do (last time)

- 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?

Kohn-Sham DFT

- Kohn-Sham approach

“The density functional can be extremized by solving a Schrödinger-like problem...”

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

$$\rho(x) = \sum_{k=1}^N |\varphi_k(x)|$$

- Kohn-Sham equations

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

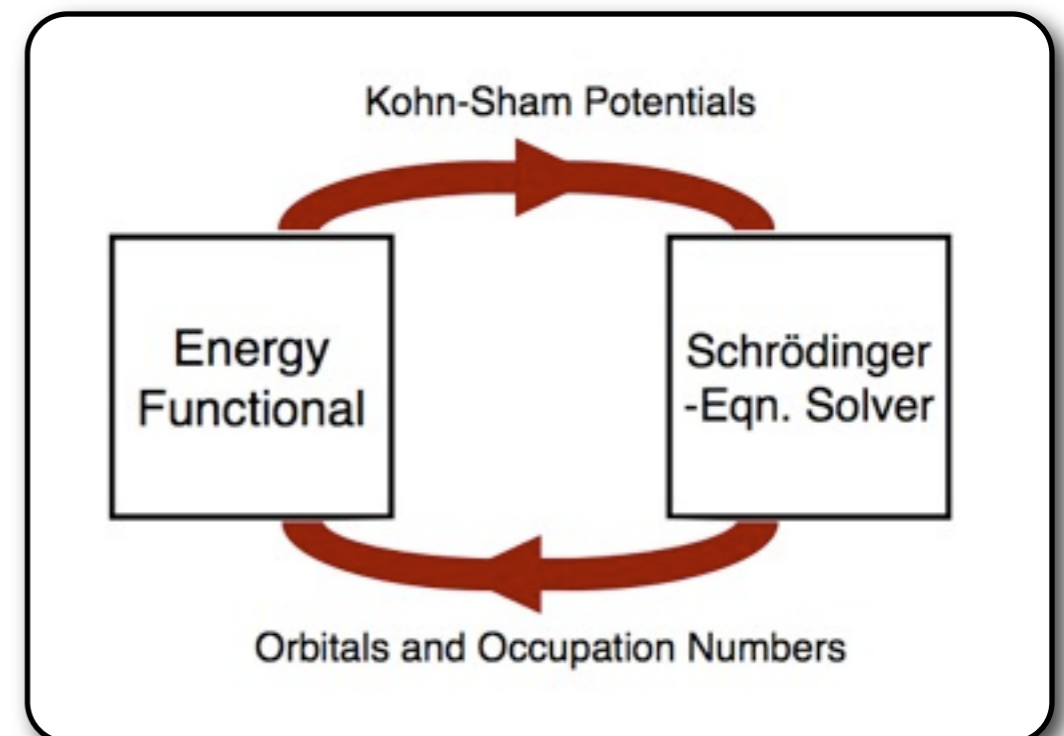
KS orbitals

KS potential

$$v_{KS}(\mathbf{r}) = \frac{\delta E_{\text{int}}[\rho]}{\delta \rho(\mathbf{r})}$$

- Solve recursively:

- Start with guess for orbitals
- Compute potential
- Solve for orbitals
- ⋮



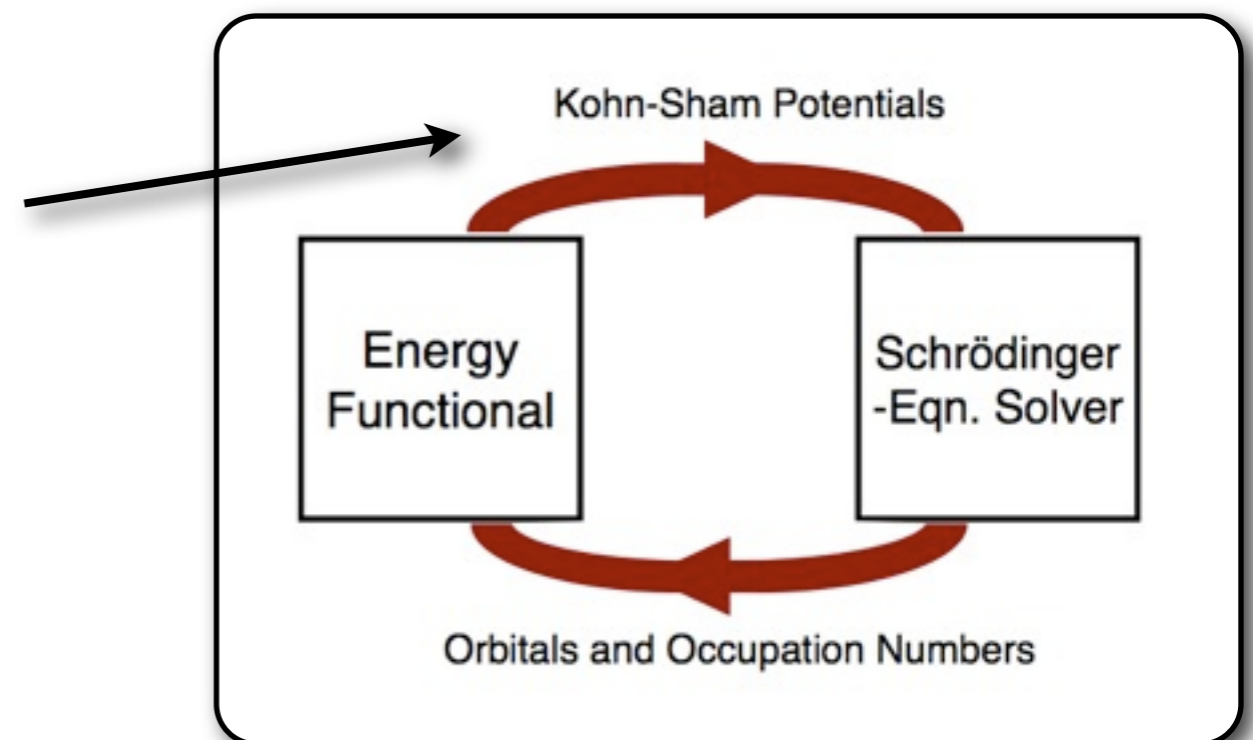
The Optimized Effective Potential

- The OEP is just the KS auxiliary potential. It is called OEP when the functional depends only implicitly on the density and explicitly on the KS orbitals.

So we can't just do this:
$$v_{KS}(\mathbf{r}) = \frac{\delta E_{int}[\rho]}{\delta \rho(\mathbf{r})}$$

Instead we have to solve an integral equation to find the potential, but other than that the KS loop remains unchanged.

 We need an OEP solver



The OEP equation

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

$\varphi_i(x)$ Kohn-Sham orbitals

$\psi_i^*(x)$ Orbital shifts

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

$$\Delta_i(x) = \underline{v_{xc}(x)} - u_{xc,i}(x)$$

$$u_{xc,j}(x') = \frac{1}{\varphi_j^*(x')} \frac{\delta E_{int}}{\delta \varphi_j(x')}$$

Goal



Solving the OEP equation

- **Kümmel-Perdew** iterative solution (KP algorithm)

- Guess xc potential and compute $\psi_i^*(x)$

Kümmel-Perdew
PRL **90**, 043004 (2003)

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

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

Use
Conjugate
gradients!

- Update xc potential

$$v_{xc}^{\text{new}} = v_{xc}^{\text{old}} + cS(x) \quad S(x) = \sum_{i=1}^N \psi_i^*(x)\varphi_i(x) + c.c.$$

- 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 $\varphi_i(x)$

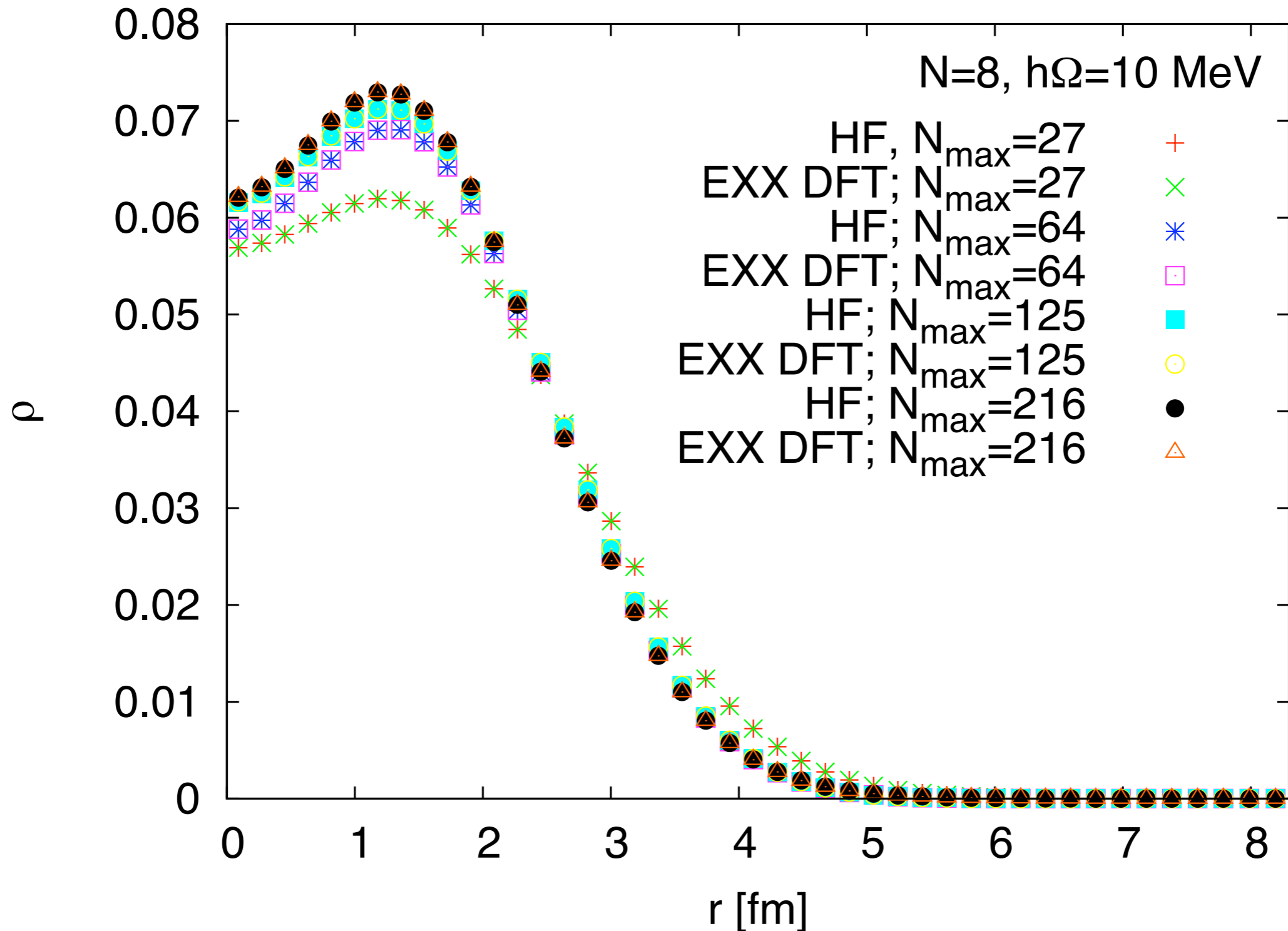
Results

- Neutron drops with the Minnesota interaction
- Various basis sizes and trap frequencies
- Full 3D problem! (no symmetry assumed)
- Exact-exchange (EXX) functional vs. Hartree-Fock
- Solved OEP Eqn. exactly with KP algorithm
- J. E. Drut and L. Platter, [arXiv:1104.4357].
Under (positive) review in Phys. Rev. C.

Results: Neutron drops

● Density profile

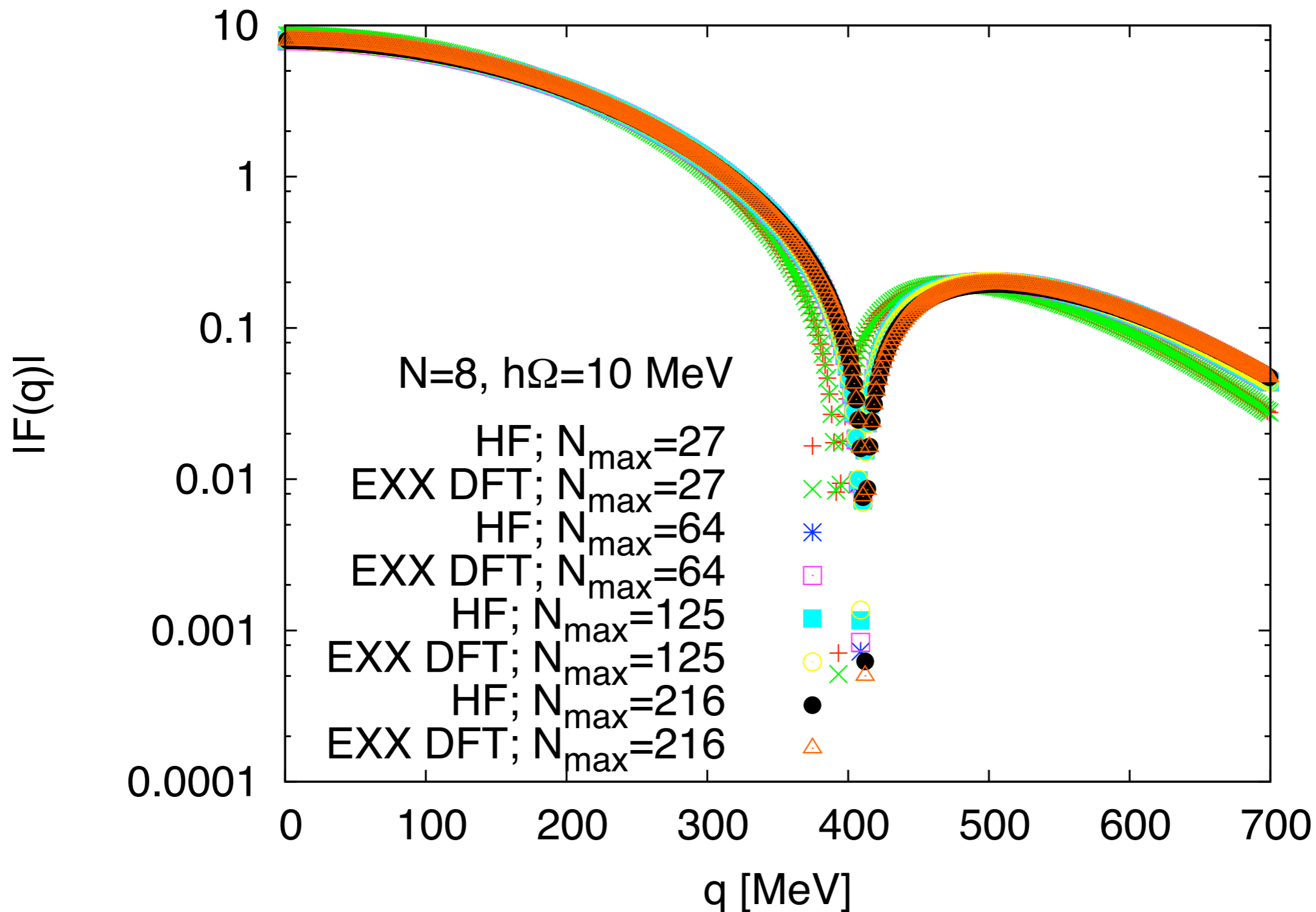
J. E. Drut and L. Platter, [arXiv:1104.4357].



Results: Neutron drops

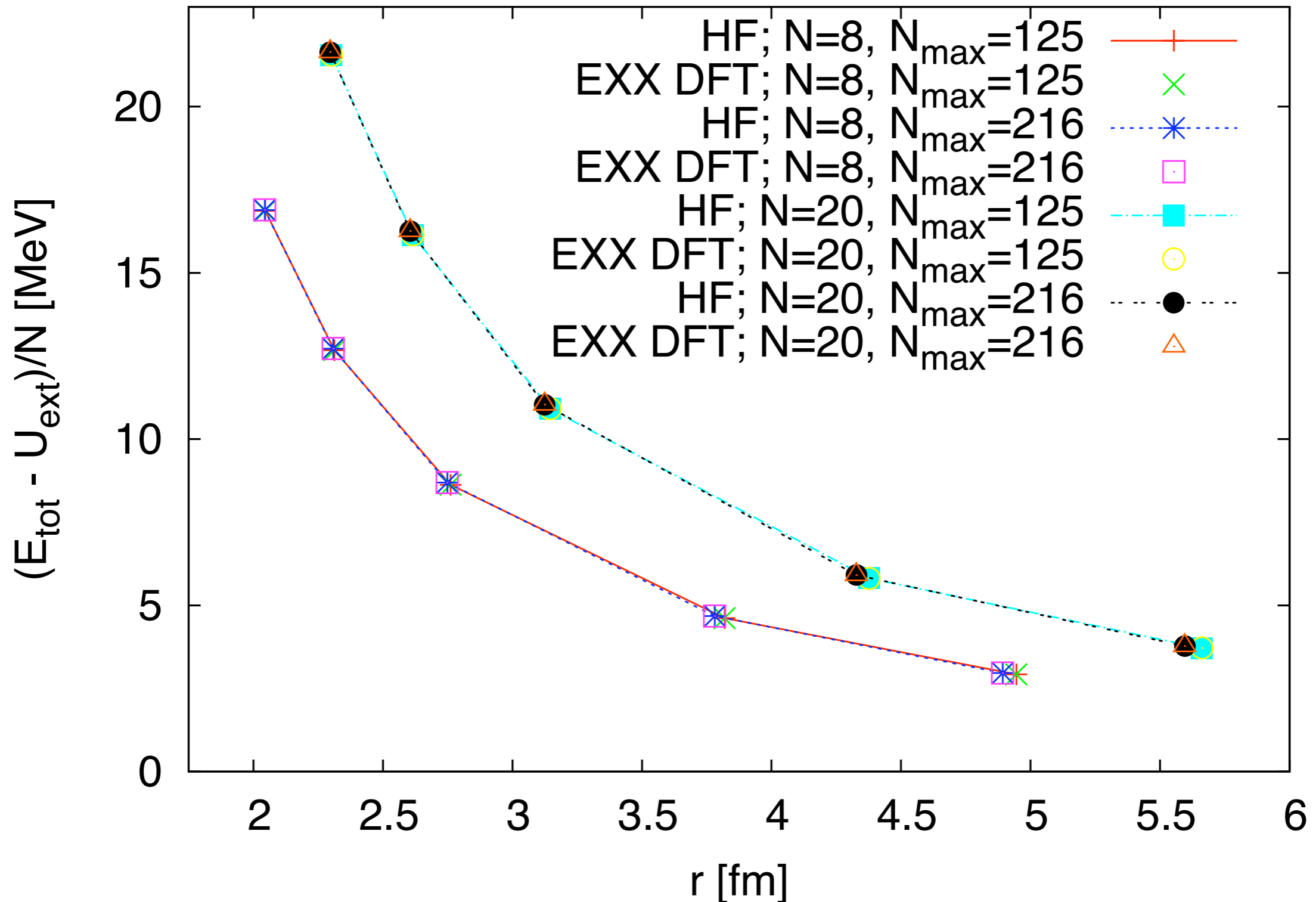
● Form factor

J. E. Drut and L. Platter, [arXiv:1104.4357].



Results: Neutron drops

- Internal energy vs. radius J. E. Drut and L. Platter, [arXiv:1104.4357].



Results: Neutron drops

- Detail

J. E. Drut and L. Platter, [arXiv:1104.4357].

TABLE I: Summary of results for the energies in MeV for Hartree-Fock (HF) and Exact-Exchange DFT (EXX), broken up into total (E_{tot}), kinetic (E_{kin}), Hartree (E_{H}), Fock (E_{F}), and internal ($E_{\text{I}} = E_{\text{tot}} - U_{\text{ext}}$). Also shown is the r.m.s. radius $\sqrt{\langle r^2 \rangle}$.

<i>Method</i>	N	$\hbar\Omega$	E_{tot}	E_{kin}	E_{H}	E_{F}	E_{I}	$\sqrt{\langle r^2 \rangle}$
HF	8	20	296.36	200.92	-225.18	159.35	135.09	2.0438
EXX	8	20	296.36	200.99	-225.24	159.39	135.14	2.0435
HF	8	10	142.43	111.22	-125.38	83.70	69.53	2.7484
EXX	8	10	142.44	111.27	-125.44	83.74	69.56	2.7478
HF	8	3	44.51	35.18	-30.51	19.05	23.72	4.8927
EXX	8	3	44.51	35.19	-30.52	19.05	23.72	4.8921
HF	20	20	941.75	707.69	-920.03	645.08	432.74	2.2965
EXX	20	20	941.77	707.83	-920.19	645.20	432.84	2.2963
HF	20	10	456.25	382.73	-488.61	326.55	220.68	3.1246
EXX	20	10	456.26	382.88	-488.80	326.69	220.77	3.1240
HF	20	3	143.52	119.55	-118.19	74.15	75.52	5.5958
EXX	20	3	143.52	119.57	-118.21	74.17	75.53	5.5954

What about pairing?

- Hartree-Fock-Bogoliubov (with **local** fields)

$$\mathcal{H}_{\text{KS}}\Phi_k(\mathbf{x}) = E_k\Phi_k(\mathbf{x})$$

$$\mathcal{H}_{\text{KS}} = \begin{pmatrix} H & D \\ D^\dagger & -H \end{pmatrix} \quad \Phi_k(\mathbf{x}) = \begin{pmatrix} u_{\uparrow,k}(\mathbf{x}) \\ u_{\downarrow,k}(\mathbf{x}) \\ v_{\uparrow,k}(\mathbf{x}) \\ v_{\downarrow,k}(\mathbf{x}) \end{pmatrix}$$

- We have to worry about renormalization issues!

(Coupling a theory to a local pairing field leads to UV divergencies)

Superfluid OEP

$$\sum_k \Psi_k^\dagger(\mathbf{x}) P_\sigma \Phi_k(\mathbf{x}) + \text{c.c.} = 0$$

$\Phi_k(\mathbf{x})$ Kohn-Sham orbitals

$$\sum_k \Psi_k^\dagger(\mathbf{x}) P_\Delta \Phi_k(\mathbf{x}) + \text{c.c.} = 0$$

$\Psi_k^\dagger(\mathbf{x})$. Orbital shifts

We just need to define some projectors:

$$P_\sigma = \begin{pmatrix} \mathbb{1}_\sigma & 0 \\ 0 & -\mathbb{1}_\sigma \end{pmatrix}$$

$$P_\Delta = \begin{pmatrix} 0 & i\sigma_2 \\ -i\sigma_2 & 0 \end{pmatrix}$$

$$\sigma_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \mathbb{1}_\uparrow = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}, \quad \mathbb{1}_\downarrow = \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}$$

Can we apply the KP algorithm here?

How can we solve it?

We can certainly determine the orbital shifts from a differential equation, as before

$$(\mathcal{H} - E_k) \Psi_k = \int d\mathbf{x}_1 \mathbf{B}_k^\dagger(\mathbf{x}, \mathbf{x}_1) \mathcal{K}_k^\dagger(\mathbf{x}_1)$$

$$\mathbf{B}_k(\mathbf{x}_2, \mathbf{x}) = \left(\Phi_k(\mathbf{x}_2) \Phi_k^\dagger(\mathbf{x}) - \mathbb{1} \delta_{\mathbf{x}\mathbf{x}_2} \right) = \sum_{q \neq k} \Phi_q(\mathbf{x}_2) \Phi_q^\dagger(\mathbf{x})$$

$$\mathcal{K}_k(\mathbf{x}) = \frac{\delta E_{\text{int}}}{\delta \Phi_k(\mathbf{x})} - \sum_{\sigma} v_{\text{KS},\sigma}(\mathbf{x}) \Phi_k^\dagger(\mathbf{x}) R^\sigma - \Delta_{\text{KS}}(\mathbf{x}) \Phi_k^\dagger(\mathbf{x}) R^\kappa$$

However, the KP approach appears to fail in this case...

How can we solve it?

$$\sum_k \Psi_k^\dagger(\mathbf{x}) P_\sigma \Phi_k(\mathbf{x}) + \text{c.c.} = 0$$

$\Phi_k(\mathbf{x})$ Kohn-Sham orbitals

$$\sum_k \Psi_k^\dagger(\mathbf{x}) P_\Delta \Phi_k(\mathbf{x}) + \text{c.c.} = 0$$

$\Psi_k^\dagger(\mathbf{x})$. Orbital shifts

Not a good measure of how the one-body fields differ from the true OEPs, everything is mixed!

 **We need a new solver!**

Alternative OEP solvers

- Self-consistent approach in coordinate space

$$v_{xc\sigma}(\mathbf{r}) = \frac{1}{2n_{\sigma}(\mathbf{r})} \sum_{i=1}^{N_{\sigma}} \left\{ |\varphi_{i\sigma}(\mathbf{r})|^2 [u_{xc\sigma}(\mathbf{r}) + (\bar{v}_{xc\sigma} - \bar{u}_{xc\sigma})] + \varphi_{i\sigma}(\mathbf{r}) \left[\left(\frac{\hbar^2}{2m} \nabla^2 + \varepsilon_{i\sigma} \right) \psi_{i\sigma}^*(\mathbf{r}) \right] \right\} + \text{c.c.}$$

- Generalized to the superfluid case
- Use Broyden's method?

- Constrained minimization with known derivatives

$$v_s^{\sigma}(\mathbf{r}) = v_{\text{ext}}(\mathbf{r}) + v_o(\mathbf{r}) + \sum_t b_t^{\sigma} g_t(\mathbf{r}),$$

Yang & Wu
PRL **89**, 143002 (2002)

$$\frac{\partial E[\{\phi_{i\sigma}\}]}{\partial b_t^{\sigma}} = \sum_{i,a \neq i} \int d\mathbf{r} \frac{\delta E[\{\phi_{i\sigma}\}]}{\delta \phi_{i\sigma}(\mathbf{r})} \phi_{a\sigma}(\mathbf{r}) \frac{\langle \phi_{a\sigma} | g_t | \phi_{i\sigma} \rangle}{\varepsilon_{i\sigma} - \varepsilon_{a\sigma}} + \text{c.c.}$$

Done / To-do update

- 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 Superfluid OEP equations (first time) ✓
- Tested EXX-DFT versus HF for 3D neutron drops with Minnesota interaction. (first time a spin-dependent potential is OEP'd!)
J. E. Drut and L. Platter, [arXiv:1104.4357]. ✓
- Improved Superfluid-OEP formalism ✓
- Coded Superfluid OEP ✓
(all parts in place, KP algorithm seems to fail in this case)

What's next?

- We have performed test calculations for the OEP with 3-body forces at the EXX level. The corresponding formalism is easy to derive. It remains to write this up and post it.
- We need to extend this to higher-body forces. The formalism is easy at the EXX level.
- We need a Superfluid OEP solver.
- Proceed towards using low-momentum potentials.
- Continue to pursue higher-order functionals (with 2-body forces for now)
- Is there a useful KLI approximation in the superfluid case?
- RPA? QRPA?

THE END

Thanks!

RPA?

- Use adiabatic connection:

Dynamic response function

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

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

$$\chi_{\text{KS}}(\vec{r}, \vec{r}', \omega) = \lim_{\eta \rightarrow 0} \sum_{\sigma=\uparrow, \downarrow} \sum_{j,k} (f_{k,\sigma} - f_{j,\sigma}) \frac{\varphi_{j,\sigma}(\vec{r}) \varphi_{k,\sigma}^*(\vec{r}) \varphi_{j,\sigma}^*(\vec{r}') \varphi_{k,\sigma}(\vec{r}')}{\omega - (\varepsilon_{j,\sigma} - \varepsilon_{k,\sigma}) + i\eta}$$

- Combine with short- and long-range splitting:

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