Analytic density functionals

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Introduction

All approaches for the calculation of density functionals from Hamiltonians describing many-body systems to date have been **numerical**.
These are based on the Kohn-Sham (KS) method [Phys. Rev. **40**, A1133 (1965)], which reduces the many-body problem to that of an effective one-body problem.

One starts with a Hamiltonian, H, from which the energy is,

$$F[\rho] = \inf_{\psi \to \rho} \langle \psi | H | \psi \rangle$$

where the wave functions are chosen under the constraint of obtaining the density. It is necessarily a many-body problem. Diagonalisation of the Hamiltonian requires,

$$\frac{\delta F}{\delta \rho} = 0.$$

One may also consider a similar definition for the kinetic energy, *viz.*,

$$G[\rho] = \inf_{\psi \to \rho} \langle \psi | T | \psi \rangle.$$

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Continuing on (with a somewhat obvious statement),

$$F = G + (F - G)$$

$$\frac{\delta F}{\delta \rho} = 0 = \frac{\delta G}{\delta \rho} + \frac{\delta (F - G)}{\delta \rho}$$

$$= \frac{\delta G}{\delta \rho} + u,$$

where we have identified the potential,

$$u = \frac{\delta (F - G)}{\delta \rho}.$$

This reduces the many-body problem to an effective one-body problem.

Normal calculations of the density functional, found in this fashion, can only be done numerically.

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Questions:

1. Is the KS assumption, which reduces the problem in this fashion, valid?
2. Is there an analytic density functional?

Consider a basis of n orthonormal, single-particle states, $\varphi_\alpha(\mathbf{r},\sigma,\tau)$. Slater determinants, ϕ_i, made out of the s-p states for N fermions make a finite subspace. The Hamiltonian can be approximated by configuration mixing.

$$\Psi = \sum_{j=1}^{\mathcal{N}} \left(C_j + iC'_j\right)\phi_j$$

$$H_{ij} = \left\langle \phi_i \middle| H \middle| \phi_j \right\rangle .$$

The energy is

$$\eta = \sum_{i,j=1}^{\mathcal{N}} C_i H_{ij} C_j$$

$$\sum_{i=1}^{\mathcal{N}} C_i^2 = 1.$$

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The density is quadratic in the mixing coefficients,

$$\rho(\mathbf{r}) = \sum_{i,j} C_i \left\langle \phi_i \middle| a_{\mathbf{r}}^{\dagger} a_{\mathbf{r}} \middle| \phi_j \right\rangle C_j .$$

Take, as an expansion set, a complete, orthonormal set of "vanishing average" functions:

$$\{S_\nu(\mathbf{r})\}, \nu = 1, \ldots, \infty$$
$$\int d\mathbf{r}\; S_\nu(\mathbf{r}) = 0, \forall \nu,$$
$$\int d\mathbf{r}\; S_\mu(\mathbf{r}) S_\nu(\mathbf{r}) = \delta_{\mu\nu}, \forall \mu, \nu .$$

We take the density with respect to some reference density, to obtain a difference

$$\Delta\rho = \rho - \rho_0 ,$$

from which we obtain the Fourier coefficients

$$\begin{aligned} \Delta_\nu &= \int d\mathbf{r}\; S_\nu(\mathbf{r}) \Delta\rho(\mathbf{r}) \\ &= \sum_{i,j} C_i \left[\int d\mathbf{r}\; S_\nu(\mathbf{r}) \left\langle \phi_i \middle| a_{\mathbf{r}}^{\dagger} a_{\mathbf{r}} \middle| \phi_j \right\rangle \right] C_j - \rho_{0\nu} . \end{aligned}$$

These define the density, as

$$\rho = \rho_0 + \sum_{i=1}^{\infty} \Delta_\nu S_\nu ,$$

$$\rho_{0\nu} = \int d\mathbf{r}\; S_\nu(\mathbf{r})\rho_0(\mathbf{r}).$$

Consider, once more,

$$\Delta_\nu = \int d\mathbf{r}\; S_\nu(\mathbf{r})\Delta\rho(\mathbf{r})$$
$$= \sum_{i,j} C_i \Big[\int d\mathbf{r}\; S_\nu(\mathbf{r}) \big\langle \phi_i \big| a_{\mathbf{r}}^\dagger a_{\mathbf{r}} \big| \phi_j \big\rangle \Big] C_j - \rho_{0\nu}.$$

Taking these, and the energies,

$$\eta = \sum_{i,j=1}^{\mathcal{N}} C_i H_{ij} C_j$$

$$\sum_{i=1}^{\mathcal{N}} C_i^2 = 1,$$

eliminates the last $(\mathcal{N}'+1)$ coefficients.

This leaves a polynomial

$$\mathcal{R}\left(\eta,\Delta_1,\ldots,\Delta_{\mathcal{N}'},C_1,\ldots,C_{\mathcal{N}-\mathcal{N}'-1}\right)=0.$$

The energy must be minimized with respect to the remaining coefficients,

$$\frac{\partial\mathcal{R}}{\partial C_i}=0,\ i=1,\ldots,\mathcal{N}-\mathcal{N}'-1$$

$$\Rightarrow \mathcal{E}\left(\eta,\Delta_1,\ldots,\Delta_{\mathcal{N}'}\right)=0.$$

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This last polynomial is the analytic (or algebraic) density functional.

Simple considerations.

Let $\mathcal{H}$ be the matrix representing the Hamiltonian on an orthonormal basis, and let $\mathcal{D}_1$ and $\mathcal{D}_2$ be the matrices representing two constraints parameterizing the density [eg. $(\Delta_\nu + \rho_{0\nu})$]. A polynomial in $\varepsilon, \lambda_1, \lambda_2$ results:

$$P(\varepsilon, \lambda_1, \lambda_2) \equiv \det\left(\mathcal{H} - \lambda_1 D_1 - \lambda_2 D_2\right) = 0.$$

ε is the free energy, λ_1, λ_2 are Lagrange multipliers. From this,

$$\frac{\partial \varepsilon}{\partial \lambda_i} = -D_i$$

$$= -\left(\frac{\partial P}{\partial \lambda_i}\right)\left[\frac{\partial P}{\partial \varepsilon}\right]^{-1}$$

$$D_i \equiv \langle D_i \rangle, i = 1,2,$$

leading to two more polynomials,

$$Q_i(D_i, \varepsilon, \lambda_1, \lambda_2) \equiv \frac{\partial P}{\partial \varepsilon} D_i - \frac{\partial P}{\partial \lambda_i} = 0.$$

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Now

$$\varepsilon = \eta - \lambda_1 D_1 - \lambda_2 D_2$$
$$\eta \equiv \langle H \rangle,$$

from which, by a process of elimination,

$$\mathcal{E}\left(\eta, D_1, D_2\right) = 0,$$

which generates the analytic DF.

Toy model

To illustrate the utility of the method, we consider a system of two fermions, whose Hamiltonian may be constructed as

$$H = T + V$$

$$T = -\frac{1}{2}\left(\frac{d^2}{dr_1^2} + \frac{d^2}{dr_2^2}\right) + \frac{1}{2}\left(r_1^2 + r_2^2\right)$$

$$\left\langle r_1 r_2 \middle| V \middle| r_1' r_2' \right\rangle = -\frac{V_0}{\sqrt{2\pi}}\delta\left[\frac{1}{2}\left(r_1 + r_2 - r_1' - r_2'\right)\right] e^{\left[\left(r_2^2 - r_1^2\right)^2 + \left(r_2'^2 - r_1'^2\right)^2\right]/4} \left(r_2 - r_1\right)\left(r_2' - r_1'\right).$$

We utilise the first four harmonic oscillator wave functions, $\varphi_0, \ldots, \varphi_3$, creating a basis of four negative-parity Slater determinants:

$$\{\varphi_0, \varphi_1\}, \{\varphi_0, \varphi_3\}, \{\varphi_2, \varphi_1\}, \{\varphi_2, \varphi_3\}$$

Choosing, $V_0 = 3$, and constraining the Hamiltonian by the second moment operator, $\left(r_1^2 + r_2^2\right)$,

$$\mathcal{H} = \begin{bmatrix} -1 & 0 & 0 & 0 \\ 0 & 7/4 & 3\sqrt{3}/4 & 0 \\ 0 & 3\sqrt{3}/4 & 7/4 & 0 \\ 0 & 0 & 0 & 45/8 \end{bmatrix}$$

$$\mathcal{D} = \begin{bmatrix} 2 & \sqrt{3/2} & 1/\sqrt{2} & 0 \\ \sqrt{3/2} & 4 & 0 & 1/\sqrt{2} \\ 1/\sqrt{2} & 0 & 4 & \sqrt{3/2} \\ 0 & 1/\sqrt{2} & \sqrt{3/2} & 6 \end{bmatrix}$$

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The polynomials read

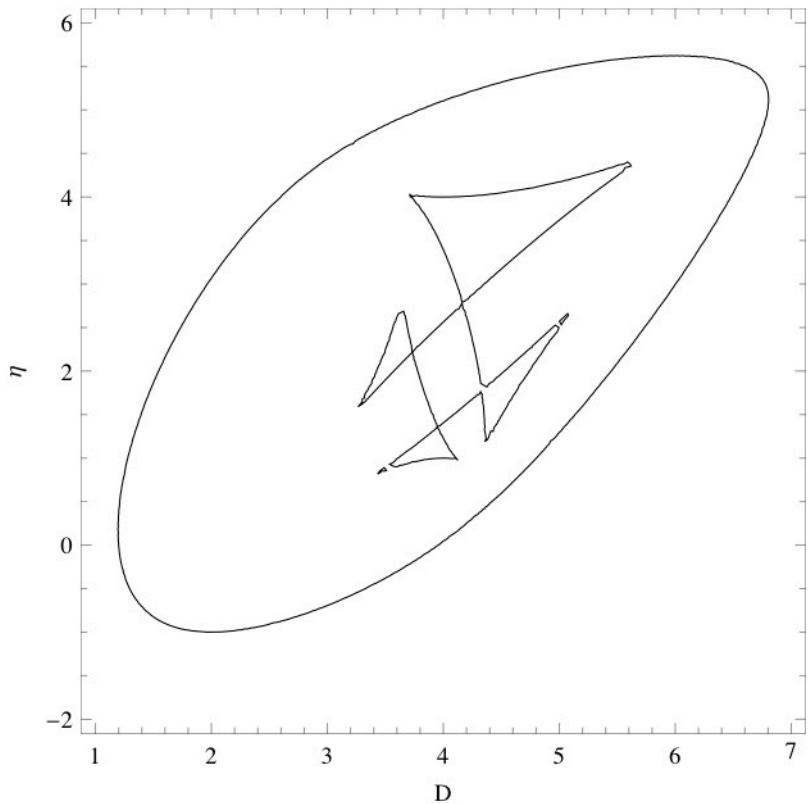
$$
\begin{aligned}
P_{\text{toy}}(\varepsilon,\lambda) &= -360+154\varepsilon+344\varepsilon^2-154\varepsilon^3+16\varepsilon^4+1464\lambda \\
&\quad +1692\varepsilon\lambda-1636\varepsilon^2\lambda+256\varepsilon^3\lambda+725\lambda^2-5140\varepsilon\lambda^2 \\
&\quad +1408\varepsilon^2\lambda^2-4192\lambda^3+3072\varepsilon\lambda^3+2064\lambda^4 \\
&= 0, \\
Q_{\text{toy}}(D,\varepsilon,\lambda) &= -1464-1692\varepsilon+1636\varepsilon^2-256\varepsilon^3-1450\lambda \\
&\quad +10280\varepsilon\lambda-2816\varepsilon^2\lambda+12576\lambda^2-9126\varepsilon\lambda^2-8256\lambda^3 \\
&\quad +\left(154+688\varepsilon-462\varepsilon^2+64\varepsilon^3+1692\lambda-3272\varepsilon\lambda+768\varepsilon^2\lambda-5140\lambda^2+2816\varepsilon\lambda^2+3072\lambda^3\right)D \\
&= 0.
\end{aligned}
$$

With the substitution $\varepsilon=\eta-\lambda D$ we have for the DF

$$\mathcal{E}_{\text{toy}}(\eta,D)=0.$$

This is 12th order in both η and D.

Contour of $\mathcal{E}_{\text{toy}}(\eta, D) = 0.$



Ground state:

$$D = 2, \eta = -1$$

Eigenvalues:

$$\mathcal{H} : 45/8, -1$$

$$\mathcal{D} : 4 \pm \sqrt{4 + \sqrt{15}}$$

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Potential energy

There is also a polynomial relating the potential energy to the constraints. Take the Hamiltonian as

$$H = h + V$$
$$V = -V_0 \mathcal{V}.$$

V_0 is an interaction strength, and may be considered a Lagrange multipler. A polynomial may be obtained:

$$\mathcal{F}\left(\langle h\rangle, \langle \mathcal{V}\rangle, D_1, \ldots, D_{\mathcal{N}'}\right)$$
$$\Rightarrow \frac{\partial \langle h\rangle}{\partial \langle \mathcal{V}\rangle} = V_0$$
$$\Rightarrow \mathcal{G}\left(V_0, \langle h\rangle, \langle \mathcal{V}\rangle, D_1, \ldots, D_{\mathcal{N}'}\right) \equiv V_0 \frac{\partial \mathcal{F}}{\partial \langle h\rangle} - \frac{\partial \mathcal{F}}{\partial \langle \mathcal{V}\rangle} = 0.$$

We can replace $\langle h\rangle \rightarrow \eta + \langle \mathcal{V}\rangle V_0$.

Eliminate η and V_0 between $\mathcal{E}$ and $\mathcal{F}, \mathcal{G}$. This provides links from the potential to the D_i. A similar approach may be utilised to construct a polynomial strictly for the kinetic energy.

Kohn-Sham considerations

The theory presented bypasses completely Kohn-Sham. KS can be illustrated by considering a basis of single-particle states, $\varphi_\alpha, \alpha = 1,\ldots,n$, from which a Slater determinant, of N orthonormal orbitals is constructed.

Orbitals	$\psi_\gamma = \sum_{\alpha=1}^{n} c_{\gamma\alpha}\varphi_\alpha$
Hamiltonian	$H = T + V$
Kinetic	$T_{\alpha\beta} = \langle \varphi_\alpha \vert T \vert \varphi_\beta \rangle$
Potential	$V_{\alpha\beta\gamma\delta} = \langle \varphi_\alpha \varphi_\beta \vert V \vert \varphi_\gamma \varphi_\delta \rangle$

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Toy model II

We construct a Slater determinant, Φ, from one positive parity and one negative parity orbital, constructed from the first 4 oscillator wave functions, $\varphi_0,\ldots,\varphi_3$:

$$\Psi_+ = t\varphi_0 + u\varphi_2$$
$$\Psi_- = v\varphi_1 + w\varphi_3.$$

This choice ensures orthogonality. Trigonometric transformation in the coefficients:

$$t = \frac{1-a^2}{1+a^2}, u = \frac{2a}{1+a^2}$$
$$v = \frac{1-b^2}{1+b^2}, w = \frac{2b}{1+b^2}$$

Density

The density is a Gaussian modulated by a polynomial of the coordinate,

$$|\Psi_+|^2 + |\Psi_-|^2 = \rho(r) = \frac{e^{-r^2}}{\sqrt{\pi}}\left(a_6 r^6 + a_4 r^4 + a_2 r^2 + a_0\right).$$

Normalisation

$$\int_{-\infty}^{\infty} \rho(r)\,dr = \frac{15}{8}a_6 + \frac{3}{4}a_4 + \frac{1}{2}a_2 + a_0 = 2.$$

There are only two independent coefficients.
The density constraint, $\Phi \Rightarrow \rho$, gives

$$4w^2/3 = a_6$$
$$t^2 - \sqrt{2}tu + u^2/2 = a_0$$
$$2u^2 + 4\sqrt{2/3}vw - 4w^2 = a_4$$
$$2\sqrt{2}tu - 2u^2 + 2v^2 - 2\sqrt{6}vw + 3w^2 = a_2$$

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In terms of a and b

$$a_6 = \frac{16b^2}{3\left(1+b^2\right)^2},\ a_0 = \frac{1-2\sqrt{2}a+2\sqrt{2}a^3+a^4}{\left(1+a^2\right)^2},$$

$$\begin{aligned}
3a_4\left(1+a^2\right)^2\left(1+b^2\right)^2/8 &= 3a^2+\sqrt{6}b+2\sqrt{6}a^2b+\sqrt{6}a^4b-6b^2-6a^2b^2 \\
&\quad -6a^4b^2-\sqrt{6}b^3-2\sqrt{6}a^2b^3-\sqrt{6}a^4b^3+3a^2b^4, \\
a_2\left(1+a^2\right)^2\left(1+b^2\right)^2/2 &= 1+2\sqrt{2}a-2a^2-2\sqrt{2}a^3+a^4-2\sqrt{6}b-4\sqrt{6}a^2b \\
&\quad -2\sqrt{6}a^4b+4b^2+4\sqrt{2}ab^2-4\sqrt{2}a^3b^2+4a^4b^2+2\sqrt{6}b^3 \\
&\quad +4\sqrt{6}a^2b^3+2\sqrt{6}a^4b^3+b^4+2\sqrt{2}ab^4-2a^2b^4-2\sqrt{2}a^3b^4+a^4b^4
\end{aligned}$$

We select a_6 and a_0 as the independent parameters, and eliminate a,b

$$\begin{aligned}
0 &= 256-1024a_0+1536a_0^2+256a_0^4-768a_4+1792a_0a_4-1280a_0^2a_4 \\
&\quad +256a_0^3a_4+864a_4^2-960a_0a_4^2+352a_0^2a_4^2-432a_4^3+144a_0a_4^3+81a_4^4-4680a_6 \\
&\quad +3840a_0a_6-2048a_0^2a_6+768a_0^3a_6+8640a_4a_6-6192a_0a_4a_6+2112a_0^2a_4a_6 \\
&\quad -5184a_4^2a_6+1296a_0a_4^2a_6+972a_4^3a_6+25056a_6^2-10944a_0a_6^2+1824a_0^2a_6^2 \\
&\quad -22032a_4a_6^2+4752a_0a_4a_6^2+5346a_4^2a_6^2-38880a_6^3+6480a_0a_6^3+14580a_4a_6^3 \\
&\quad +18225a_6^4
\end{aligned}$$

The Slater energy is

$$\begin{aligned}\eta &\equiv \langle \Phi | H | \Phi \rangle \\ &= \left(t^2 + 5u^2 + 3v^2 + 7w^2\right)/2 - V_0\left[2\left(4t^2 + u^2\right)v^2 - 4\sqrt{3}tuvw + \left(6t^2 + u^2\right)w^2\right]/8 \\ &= \left[2 + 12a^2 + 2a^4 + 12b^2 + 40a^2b^2 + 12a^4b^2 + 2b^4 + 12a^2b^4 + 2a^4b^4\right. \\ &\quad -V_0\left(1 - a^2 + a^4 - 2\sqrt{3}a^3b + b^2 - 2a^2b^2 + a^4b^2 + 2\sqrt{3}ab^3 - 2\sqrt{3}a^3b^3\right. \\ &\quad \left.\left. + b^4 - a^2b^4 + a^4b^4\right)\right] / \left[\left(1 + a^2\right)\left(1 + b^2\right)\right]^2 .\end{aligned}$$

The DF is constrained now by

$$\begin{aligned}\mathcal{F}[\rho] &= \min_{\Phi \Rightarrow \rho} \langle \Phi | H | \Phi \rangle \\ &= \min_{\Phi \Rightarrow a_6} \langle \Phi | H | \Phi \rangle .\end{aligned}$$

For the ground state, a_6=0, (no halo), and b is eliminated. This leaves the precursor…

$$
\begin{aligned}
&\mathcal{P}(\eta, a_6, a) = 0 \\
&= 1024 + 12288a^2 + 38912a^4 + 12288a^6 + 1024a^8 \\
&+1536a_6 + 12288a^8a_6 + 21504a^4a_6 + 12288a^6a_6 \\
&+1536a^8a_6 + 576a_6^2 + 2304a^2a_6^2 + 3456a^4a_6^2 + 2304a^6a_6^2 \\
&+576a^8a_6^2 - 1024\eta - 8192a^2\eta - 14336a^4\eta - 8192a^6\eta \\
&-1024a^8\eta - 768a_6\eta - 3072a^2a_6\eta - 4608a^4a_6\eta - 3072a^6a_6\eta \\
&-768a^8a_6\eta + 256\eta^2 + 1024a^2\eta^2 + 1536a^4\eta^2 + 1024a^6\eta^2 \\
&+256a^8\eta^2 - 1024V_0 - 5120a^2V_0 + 4096a^4V_0 - 5120a^6V_0 \\
&-1024a^8V_0 - 576a_6V_0 + 384a^2a_6V_0 + 384a^4a_6V_0 \\
&+384a^6a_6V_0 - 576a^8a_6V_0 + 144a_6^2V_0 + 288a^2a_6^2V_0 \\
&+288a^4a_6^2V_0 + 288a^6a_6^2V_0 + 144a^8a_6^2V_0 + 512\eta V_0 \\
&+512a^2\eta V_0 + 512a^6\eta V_0 + 512a^8\eta V_0 - 96a_6\eta V - 192a^2a_6\eta V_0 \\
&-192a^4a_6\eta V_0 - 192a^6a_6\eta V_0 - 96a^8a_6\eta V_0 + 256V_0^2 \\
&-512a^2V_0^2 + 768a^4V_0^2 - 512a^6V_0^2 + 256a^8V_0^2 \\
&-96a_6V_0^2 - 480a^2a_6V_0^2 + 960a^4a_6V_0^2 - 480a^6a_6V_0^2 \\
&-96a^8a_6V_0^2 + 9a_6^2V_0^2 + 432a^2a_6^2V_0^2 - 846a^4a_6^2V_0^2 \\
&+432a^6a_6^2V_0^2 + 9a^8a_6^2V_0^2
\end{aligned}
$$

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Energy minimsation, with respect to a:

$$\mathcal{Q} \equiv \frac{\partial \mathcal{P}}{\partial a} = 0$$
$$= \left(32 + 24a_6 - 16\eta - 16V_0 + 3a_6V_0\right)\left(128 + 48a_6 - 32\eta - 8V_0 + 3a_6V_0\right)$$
$$\times\left(4096 + 4608a_6 + 1152a_6^2 - 3072\eta - 1536a_6\eta + 512\eta^2 - 2304V_0\right.$$
$$\left.-480a_6V_0 + 216a_6^2V_0 + 640\eta V_0 - 144a_6\eta V_0 + 128V_0^2 - 144a_6V_0^2 + 63a_6^2V_0^2\right)$$

Minimisation with respect to a_6

$$\mathcal{S} \equiv \frac{\partial \mathcal{Q}}{\partial a_6} = 0$$
$$= \left(\eta + V_0 - 2\right)\left(4\eta + V_0 - 16\right)\left(8\eta + V_0 - 48\right)\left(4\eta + 3V_0 - 16\right)$$
$$\times\left(64 + 36V_0 - 2\eta V_0 + V_0^2\right)$$
$$\times\left(-1024 - 1152V_0 + 64\eta V_0 + 316V_0^2 - 348\eta V_0^2 + 47\eta^2V_0^2 - 264V_0^3 + 52\eta V_0^3 + 5V_0^4\right)$$

Combining these two equations gives the condition for a_6:

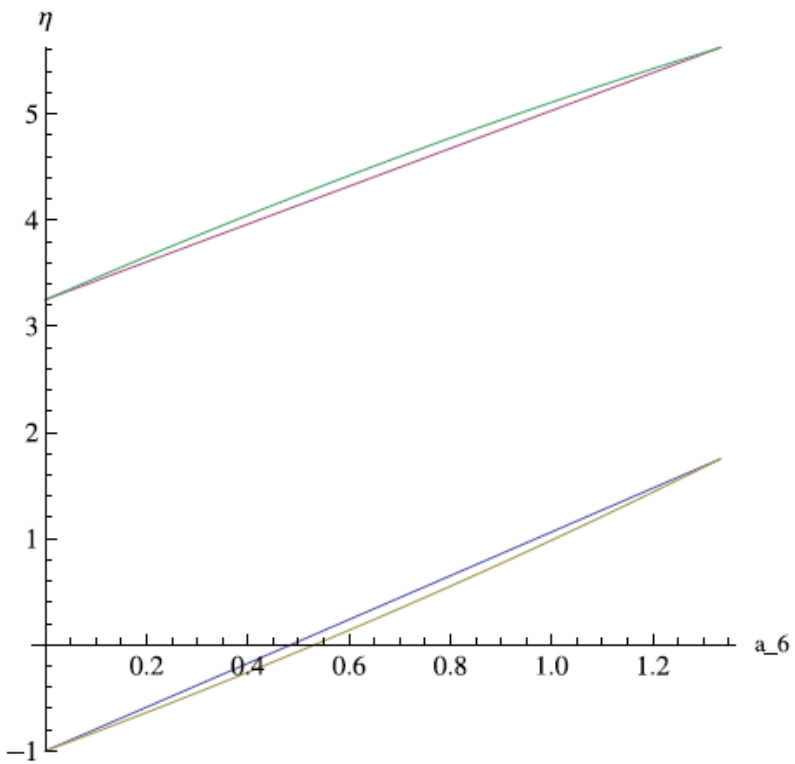
$$a_6\left(3a_6-4\right)\left(3a_6V_0-24V_0-64\right)\left(524288+491520V_0-49512a_6V_0\right.$$
$$+151552V_0^2+46080a_6V_0^2-54144a_6^2V_0^2+18432V_0^3+7680a_6V_9^3$$
$$\left.-10152a_6^2V_0^3+3024a_6V_0^4-2961a_6^2V_0^4\right)=0.$$

We set $V_0=3$ as before, whence,

$$\left(16-33a_6+16\eta\right)\left(104+57a_6-32\eta\right)$$
$$\left(-1664+1872a_6+2367a_6^2-1152\eta-1968a_6\eta+512\eta^2\right)=0.$$

Lowest root: $\eta=-2.98623$, spurious, as it gives a negative value for a_6.

Allowed values for η



$$\eta = -1$$
$$a_6 = 0$$
$$\Rightarrow b = 0$$
$$\Rightarrow a = 0$$
$$a_0 = 1$$
$$a_4 = 0$$
$$a_2 = 2$$

Hence, the optimal density,

$$\rho = \frac{\left(1+2r^2\right)e^{-r^2}}{\sqrt{\pi}}.$$

Consider a truncated subspace on some finite single particle basis for a system of N particles with projector $\mathcal{P}$.

Hamiltonian: $\mathcal{P}H\mathcal{P}$

One-body Hamiltonian: $H_0 = T + W_0$

$$W_0 = \sum_{i=1}^{N} w_0(r_i)$$

Ground state density: $\Phi_0 \Rightarrow \rho_0$

Difference: $\Delta\rho = \rho - \rho_0$

$$= \sum_{\beta=1}^{\infty} b_\beta S_\beta(r)$$

Given a Hamiltonian, H_0, the polynomial method returns $\mathcal{K}(\kappa, b_1, \ldots, b_{\mathcal{N}'})$.

For which, for the lowest root of $\mathcal{K} = 0$,

$$\kappa' = \min_{\Phi \Rightarrow b_1, \ldots, b_{\mathcal{N}'}} \langle \Phi | H_0 | \Phi \rangle .$$

For the full Hamiltonian, one gets a polynomial and constrained minimum for the lowest root,

$$\mathcal{E}(\eta, b_1, \ldots, b_{\mathcal{N}'}),$$

$$\eta' = \min_{\Psi \Rightarrow b_1, \ldots, b_{\mathcal{N}'}} \langle \Psi | H | \Psi \rangle .$$

Difference: $\Omega(\omega; b_1, \ldots, b_{\mathcal{N}'}); \omega = \eta - \kappa$

Diagonalisation of $\mathcal{P}H\mathcal{P} \Rightarrow \frac{\partial \kappa}{\partial b_\beta} + \frac{\partial \omega}{\partial b_\beta} = 0, \ \beta = 1, \ldots \mathcal{N}'$

One-body potential: $v_\beta = -\frac{\partial \Omega}{\partial b_\beta} \frac{\partial \omega}{\partial \Omega}$

$$v_\Delta(r) = \sum_{\beta=1}^{\mathcal{N}'} v_\beta S_\beta(r).$$

Φ is the ground state of $\mathcal{P}\left[H_0 + \sum_{i=1}^{N} v_\Delta(r_i)\right]\mathcal{P}$. Note:

$$\left\langle \Phi \middle| \mathcal{P} S_\beta \mathcal{P} \middle| \Phi \right\rangle = \left\langle \Phi \middle| S_\beta \middle| \Phi \right\rangle$$

Energy derivatives:

$$\frac{\partial E}{\partial v_\beta} = \int \left(r^{d-2} dr\right)\left(\Delta\rho + \rho_0\right) S_\beta$$

$$= b_\beta + b_0$$

Kohn-Sham potential: $\mathcal{P}\left(w_0 + v_\Delta\right)\mathcal{P}$

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- The properties of concavity are explicitly contained in the method.
- Potential and kinetic energies are easily obtainable.
- Kohn-Sham can be recovered.