Guaranteed convergence of a regularized Kohn–Sham iteration in finite dimensions

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The exact Kohn–Sham iteration of generalized density-functional theory in finite dimensions with Moreau–Yosida regularized universal Lieb functional and an adaptive damping step is shown to converge to the correct ground-state density.

The ubiquitous Kohn–Sham (KS) scheme \cite{1} of ground-state density-functional theory (DFT) is the cornerstone of electronic structure calculations in quantum chemistry and solid-state physics. This scheme maps a complicated system of interacting electrons to an auxiliary, non-interacting Kohn–Sham system. Thereby it gives a set of coupled one-particle equations that need to be solved self consistently. Since a direct solution is unfeasible, practical approaches are variations of self-consistent field methods taking the form of fixed-point iterations or of energy minimization algorithms \cite{2–7}. To date, no iterative method has been rigorously shown to converge to the correct ground-state density. Convergence results for approximate schemes are available \cite{8}, but reliably achieving convergence in systems with small band gaps or for transition metals remains a hard practical challenge \cite{9}. Hence, a method with mathematically guaranteed convergence is of central importance.

An early insight is that iterations commonly fail unless oscillations between trial states are damped \cite{2}. Work by Cancès and Le Bris \cite{10,11} lead to the optimal damping algorithm (ODA) based on energy minimization by line-search along a descent direction. Wagner et al. \cite{12,13} presented a similar scheme and claimed to have proven convergence in the setting of exact DFT, while only the strict descent of energies was secured. This issue was addressed in Laestadius et al. \cite{14} where a similar iterative scheme was proposed that proved a weak type of convergence after Moreau–Yosida (MY) regularization to ensure differentiability of the universal Lieb functional \cite{15}. Such a regularized DFT has been previously suggested by Kvaal et al. \cite{16}. Weak-type convergence here means that the energy converges to an upper bound for the exact energy. A rich study of possible strategies for self-consistent field iteration was recently put forward by Lammert \cite{17}. Yet in all those works the question of a limit density and corresponding KS potential was still left open. On the other side, the result in Laestadius et al. \cite{14} is fully applicable to not only the setting of standard DFT, but to all DFT-flavors that fit into the given framework of reflexive Banach spaces. It has already been successfully applied to paramagnetic current DFT (CDFT) \cite{18}. This general approach that reaches beyond standard DFT is followed also in this letter.

In what follows we give a fully rigorous proof of convergence for the exact KS iteration scheme in a finite-dimensional state space. Due to the techniques involved, the new iteration scheme was baptized “MYKSODA” in Laestadius et al. \cite{18}. The version given here includes a different, more conservative damping step that helps to prove convergence. To distinguish the two versions, we denote them “MYKSODA-S” for shorter, conservative steps, and “-L” for the original longer steps. The selection of the damping critically depends on MY regularization that makes the curvature of the universal Lieb functional bounded above. The convergence speed is increased by a larger regularization factor $\varepsilon$ which corresponds to a smaller allowed curvature. The reason why a large $\varepsilon$ is not desirable lies in numerical accuracy and the availability of good approximation functionals.

We will now present the mathematical framework. For a much more detailed discussion of generalized KS iteration schemes in Banach spaces that can also be infinite dimensional we refer to Laestadius et al. \cite{14}. The spaces for densities and potentials are chosen to be the Hilbert space $X = X^\ast = L^2(M)$, $M \in \mathbb{N}$, which corresponds to a finite one-particle basis, a lattice system with $M$ sites, or many other possible settings. The reason for this dual choice of spaces is how densities and potentials couple in the energy expression. What is denoted $\int_X v \rho \, dx$ in standard DFT is $\langle v, \rho \rangle$ with $\rho \in X$, $v \in X^\ast$ in our generalized setting. For the internal energy (kinetic and interaction) of the full system a universal functional $\tilde{F}$, like the one defined by constrained search \cite{15,19} over all $N$-particle density matrices $\Gamma$ that yield a given density $\rho \in X$, is
introduced,
\[ \tilde{F}(\rho) = \inf_{\Gamma \to \rho} \{ \text{Tr}(\mathcal{H}_{\text{kin}} + \mathcal{H}_{\text{int}}) \Gamma \}. \] (1)

Here \( \mathcal{H}_{\text{kin}} \) stands for the kinetic energy contribution to the Hamiltonian and \( \mathcal{H}_{\text{int}} \) for interactions. Consequently the functional \( \tilde{F} \) is defined on a set \( \tilde{X} \subset X \) of physical densities that come from an \( N \)-particle density matrix (ensemble \( N \)-representability). This set \( \tilde{X} \) will be assumed bounded in \( X \). Since all physical densities are normalized in the \( L^1 \) norm and all norms are equivalent in finite dimensions this follows naturally. It also holds for CDFT on a finite lattice, since the current density is bounded by the hopping parameter [20 Eq. (25)], and for one-body reduced density matrix functional theory (RDMFT) in finite basis sets, since the off-diagonal elements of the reduced density matrix are bounded by the diagonal ones that give the usual density [21, Eq. (3.49)].

On the other hand, elements in \( X \) will in general not constitute physical densities. In standard DFT this means that an arbitrary \( x \in X \) does not have to be normalized or even positive. Such an \( x \in X \) will thus be called a quasi-density. We keep the notation \( \rho \) to mark out physical densities. The total energy is the infimum of \( \tilde{F}(\rho) \) plus the the potential energy coming from a given external potential \( v \in X^* \), taken over all physical densities,
\[ E(v) = \inf_{\rho \in \tilde{X}} \{ \tilde{F}(\rho) + \langle v, \rho \rangle \}. \] (2)

It is linked to a functional \( F \) on \( X \) by the Legendre–Fenchel transformation (convex conjugate). Then \( F \) can be transformed back to the same \( E \) as
\[ F(x) = \sup_{v \in X^*} \{ E(v) - \langle v, x \rangle \}, \] (3)
\[ E(v) = \inf_{x \in \tilde{X}} \{ F(x) + \langle v, x \rangle \}. \] (4)

The functional \( F \) is by construction convex and lower semi-continuous [15 Th. 3.6] and has \( F(x) = +\infty \) whenever \( x \) is not in the domain \( \tilde{X} \) of \( \tilde{F} \). Minimizers of (2) are the ground-state densities, which establishes a link to the corresponding Schrödinger equation. They stay the same if one switches from \( \tilde{F} \) to \( F \) and thus minimizers of (4) are always in \( \tilde{X} \). Finding such minimizers of (4) is equivalent to determining the superdifferential of \( E \), the set of all dual elements (quasi-densities) that yield a graph completely above \( E \),
\[ \rho \in \partial E(v) \subset \tilde{X}. \] (5)

The MY regularization of the functional \( F \) on \( X \) is defined as
\[ F_\varepsilon(x) = \inf_{y \in X} \{ F(y) + \frac{1}{\varepsilon} \| x - y \|^2 \}. \] (6)

The visual understanding of this is the following. As the vertex of the regularization parabola \( \frac{1}{\varepsilon} \| x - y \|^2 \) moves along the graph of \( F \), the regularized \( F_\varepsilon \) is given by the traced out lower envelope as visualized in Fig. 1. It also means the regularization puts an upper bound of \( \varepsilon^{-1} \) to the (positive) curvature of \( F_\varepsilon \). This will be an important ingredient in the convergence proof: A bound on the curvature means the convex functional \( F_\varepsilon \) cannot change from falling to rising too quickly, yielding a secure bound on the possible step length for descent.

The regularized \( F_\varepsilon \) is then differentiable and even has a continuous gradient \( \nabla F_\varepsilon \) (Fréchet differentiability), something that will become important too in the convergence proof, if additionally \( X^* \) is assumed uniformly convex [14 Th. 9]. Uniform convexity is trivially fulfilled in the cases of a finite dimensional, strictly convex Banach space \( X^* \) or for any Hilbert space \( X = X^* \). With \( F_\varepsilon \) we define the associated energy functional
\[ E_\varepsilon(v) = \inf_{x \in X} \{ F_\varepsilon(x) + \langle v, x \rangle \}. \] (7)

The functional in (7) is not the MY regularization of \( E \) but the Legendre–Fenchel transformation of \( F_\varepsilon \). If \( z \in X \) is a minimizer in (7), called the ground-state quasi-density, then the gradient of \( F_\varepsilon + v \) at \( z \) must be zero,
\[ \nabla F_\varepsilon(z) + v = 0. \] (8)

Since the regularized functional is differentiable everywhere, the usual problem of (non-interacting) \( v \)-representability is avoided in the regularized setting. But \( E_\varepsilon \) is still not differentiable, so we resort to the superdifferential like in (4). Since any such element \( z \in \partial E_\varepsilon(v) \) automatically solves (8) it is the ground-state quasi-density of the regularized reference system for a potential \( v \). Two important properties of \( E_\varepsilon \) are [13] Th. 10 and
which relate the regularized system back to the unregularized one. Note that the \( \varepsilon \) in \( (10) \) takes a role comparable to that of \textit{permittivity}, linking potentials to densities. Since \( E \) is already concave, the subtraction of a parabola in \( (9) \) makes \( E_\varepsilon \) strongly concave.

To set up a KS iteration scheme we define a \textit{reference system} that is non-interacting by

\[
\tilde{\tilde{F}}(\rho) = \inf_{F} \{ \text{Tr}(H_{\text{kin}}\Gamma) \}
\]

on the same \( \tilde{X} \subset X \) and define \( E_0, F_0, \) and \( E_0^0 \) analogously. The analogue of \( (8) \) for \( F_0^0 \) at the same quasi-density \( z \in X \) is

\[
\nabla F_0^0(z) + v_0^0 = 0,
\]

and defines the KS potential \( v_0^{KS} \). Simply equating \( (8) \) and \( (12) \) gives

\[
\nabla F_\varepsilon(z) + v \varepsilon = \nabla F_\varepsilon^0(z) + v_0^{KS},
\]

where the ground-state quasi-density \( z \) and the auxiliary KS potential \( v_0^{KS} \) for the reference system are still unknown and neither \( F_\varepsilon \) nor \( F_\varepsilon^0 \) has a simple, explicit expression. The trick is to determine \( z \) and \( v_0^{KS} \) in an iterative algorithm and to replace them by sequences \( x_i \to z \), \( v_i \to v_0^{KS} \). The indicated convergence is our major concern in the following proof. We get an update rule for the potential sequence \( (v_i) \), directly from \( (13) \),

\[
v_{i+1} = v + \nabla F_\varepsilon(x_i) - \nabla F_\varepsilon^0(x_i),
\]

and determine the next quasi-density by solving for the ground-state of the regularized reference system with \( v_{i+1} \). This iteration has the stopping condition \( v_{i+1} = -\nabla F_\varepsilon^0(x_i) \) which means \( v = -\nabla F_\varepsilon(x_i) \) by \( (14) \). Then \( x_i \) is already the sought-after ground-state quasi-density \( z \) and thus also \( v_{i+1} = v_0^{KS} \) is the respective KS potential yielding the same quasi-density for the reference system.

The most important ingredient of practical KS calculations enters by giving suitable approximations for the expression \( \nabla F_\varepsilon - \nabla F_\varepsilon^0 \) (Hartree-exchange-correlation (Hxc) potential including the correlated kinetic energy). For our purpose of showing convergence of exact KS theory we proceed as if this object is known. The KS algorithm is then the following: In step (a) get the new potential by \( (14) \) above. In step (b) solve the (simpler) ground-state problem for the reference system by choosing the next quasi-density from \( \partial E_\varepsilon^0(v_{i+1}) \). From \( (10) \) it follows that \( \partial E_\varepsilon^0(v_{i+1}) \) can be determined from the set of ground-state densities of the reference system, which just means solving the non-interacting Schrödinger equation. Finally, to be able to ensure a strictly descending energy and to show convergence of \( (x_i), (v_i) \), include a damping step (c) with an adaptively chosen step size.

**MYKSODA iteration scheme.** Assume \( \tilde{X} \) bounded and \( E^0 \) finite everywhere. For \( v \in X^* \) fixed, set \( v_1 = v \) and select \( x_1 \in \partial E_\varepsilon^0(v) \). Iterate \( i = 1, 2, \ldots \) according to:

(a) Select \( v_{i+1} = v + \nabla F_\varepsilon(x_i) - \nabla F_\varepsilon^0(x_i) \) and stop if \( v_{i+1} = -\nabla F_\varepsilon^0(x_i) = v_0^{KS} \).

(b) Select \( x_{i+1} \in \partial E_\varepsilon^0(v_{i+1}) \) and get the iteration direction \( y_i = (x_{i+1} - x_i)/\|x_{i+1} - x_i\| \).

(c) Choose the step length \( \tau_i = -\varepsilon(\nabla F_\varepsilon(x_i) + v, y_i) > 0 \) and set \( x_{i+1} = x_i + \tau_i y_i \).

We prove below that this algorithm guarantees convergence to the correct KS potential, \( v_i \to v_0^{KS} \), and to the quasi-density, \( x_i \to z \), of both, the full system with \( v \) and the reference system with \( v_0^{KS} \). The corresponding energy is then determined by \( E_\varepsilon(v) = F_\varepsilon(z) + (v, z) > -\infty \).

These are still solutions of the regularized problem, but with \( (9) \) and \( (10) \) a transformation back to the unregularized setting is easily achieved. This, unlike the usually assumed unregularized KS iteration, gives different ground-state densities for the non-interacting and the interacting system, while circumventing all problems of differentiability and thus of \( \rho \)-representability. The assumption that \( E^0 \) is finite everywhere is trivially fulfilled in a finite-dimensional setting because \( E^0 \) is the outcome of a finite sum of numbers. It is still kept here to connect more closely to the setting of standard DFT and CDFT, where \( E^0 \) finite can be shown to hold even in the infinite-dimensional setting, see Lieb \[15, Th. 3.1(iii)\] and Laestadius et al. \[18, Lem. 20\], respectively.

**Convergence proof.** We refer to the the first part of the proof of Theorem 12 in Laestadius et al. \[14\] to show that the superdifferential \( \partial E_\varepsilon^0(v_{i+1}) \) is everywhere non-empty because of \( E^0 \) finite, guaranteeing that the (regularized) ground-state problem in (b) always has at least one solution. The directional derivative of \( F_\varepsilon + v \) at \( x_i \) in direction \( x_{i+1}' - x_i \) can be rewritten by (a),

\[
(\nabla F_\varepsilon(x_i) + v, x_{i+1}' - x_i) = (v_{i+1} + \nabla F_\varepsilon^0(x_i), x_{i+1}' - x_i).
\]

Realizing that \( x_{i+1}' \in \partial E_\varepsilon^0(v_{i+1}) \) from (b) and \( x_i \in \partial E_\varepsilon^0(\nabla F_\varepsilon^0(x_i)) \) from invertibility \[14, Lem. 4\], we rewrite
the right hand side of (15) with the help of (10), substituting
\[
\begin{align*}
x_i^{t+1} &= x_i^t + \varepsilon v_{i+1} \in \mathcal{E}^0(E_0(v_{i+1})), \\
x_i &= x_i + \varepsilon \nabla F^0_i(x_i) \in \mathcal{E}^0(\nabla F^0_i(x_i)),
\end{align*}
\]
which gives
\[
(v_{i+1} + \nabla F^0_i(x_i), x_i^{t+1} - \hat{x}_i) - \varepsilon \|v_{i+1} + \nabla F^0_i(x_i)\|^2. \tag{18}
\]
Now since \(x_i^{t+1}, \hat{x}_i\) are selected from the superdifferential of \(E^0\) for the respective potentials \(v_{i+1}, \nabla F^0_i(x_i)\), the inner product is always smaller or equal to zero \([14, \text{Lem. 5}]\). This property is called monotonicity of \(\mathcal{E}^0\) and directly follows from concavity of \(E^0\). What follows is strong monotonicity of \(E^0\), i.e.,
\[
\langle \nabla F_i(x_i) + v, x_{i+1} - x_i \rangle \leq -\varepsilon \|v_{i+1} + \nabla F^0_i(x_i)\|^2 = -\varepsilon \|\nabla F_i(x_i) + v\|^2. \tag{19}
\]
The last line follows from (a) and is strictly smaller than zero if not \(\|\nabla F_i(x_i) + v\| = 0\), which means that we have already converged to the ground-state quasi-density. We thus infer that, unless converged, we always have a negative directional derivative of \(F_i + v\) at \(x_i\) in the step direction \(y_i\), which is parallel to \(x_{i+1} - x_i\),
\[
\langle \nabla F_i(x_i) + v, y_i \rangle < 0. \tag{20}
\]
Such a negative directional derivative means the left leg of the regularization parabola is aligned tangentially to the (differentiable) energy functional \(F_i + v\), like it is depicted in Fig. 2. The next quasi-density step \(x_{i+1} = x_i + \tau_i y_i\) is then chosen at the vertex of this regularization parabola. This chooses to a choice of step length \(\tau_i\)
\[
\frac{1}{2\varepsilon}\|x - x_{i+1}\|^2 + m_i
\]
where the directional derivatives at \(x_i\) in direction \(y_i\) of the regularization parabola \(\frac{1}{2\varepsilon}\|x - x_{i+1}\|^2\) and \(F_i + v\) are equal, which means
\[
\langle \nabla F_i(x_i) + v, y_i \rangle = -\frac{1}{\varepsilon}(x_{i+1} - x_i, y_i) = -\frac{1}{\varepsilon}\|x_{i+1} - x_i\| = -\frac{\tau_i}{\varepsilon}. \tag{21}
\]
This construction yields a \(x_{i+1} \neq x_i\) where the energy \(e_i = F_i(x_i) + \langle v, x_i \rangle\) is always larger than the energy value \(m_i\) at the vertex, see Fig. 2. Since the regularization parabola also lies fully above the energy functional \(F_i + v\) by construction, the energy \(e_{i+1}\) at \(x_{i+1}\) must obey \(e_{i+1} \leq m_i < e_i\). The strictly decreasing \(e_i\) is now by definition bounded below by \(E^0(v)\) from (7) and thus converges. By determining \(e_i - m_i\) from the regularization parabola and then combining it with (21),
\[
\frac{\tau_i^2}{2\varepsilon} = \frac{1}{2\varepsilon}\|x_{i+1} - x_i\|^2 = e_i - m_i \leq e_i - e_{i+1} \rightarrow 0, \tag{22}
\]
we can infer convergence of \((x_i)_i\). Step (a) then defines an associated potential
\[
\lim_{i \to \infty} v_{i+1} = v + \nabla F^0(x_i) - \nabla F^0_i(x_i), \tag{23}
\]
since the gradients are both continuous. After having proven that the densities and potentials converge, it shall be demonstrated that they converge indeed to the expected ground-state quasi-density, \(\rho\), and KS potential, \(v_{\text{KS}}\). We now come back to (19), where substituting
\[
x_{i+1} - x_i = y_i \|x_{i+1} - x_i\|
\]
gives
\[
\|x_{i+1} - x_i\| \langle \nabla F_i(x_i) + v, y_i \rangle \leq -\varepsilon\|\nabla F_i(x_i) + v\|^2, \tag{24}
\]
which together with (21) results in
\[
\|x_{i+1} - x_i\| \frac{\tau_i}{\varepsilon} \geq \varepsilon\|\nabla F_i(x_i) + v\|^2. \tag{25}
\]
We already know from the convergence of densities that \((x_i)_i\) is bounded, further
\[
x_{i+1} \in \mathcal{E}^0(E_0(v_{i+1})) = \mathcal{E}^0(E_0(v_{i+1}) - \varepsilon v_{i+1}) \tag{26}
\]
by (b) and (10). But \(\mathcal{E}^0(E_0(v_{i+1})) \subset \hat{X}\), which is assumed to be bounded, and \((v_i)\) converges as well. Thus \(\|x_{i+1} - x_i\|\) is bounded and since \(\tau_i \to 0\) it follows \(\|\nabla F_i(x_i) + v\| \to 0\) and \(\|\nabla F^0_i(x_i) + v_{i+1}\| \to 0\). This in turn means \(v = -\nabla F_i(x)\) so \(\lim x_i = z\) is the ground-state quasi-density for the potential \(v\) in the full, regularized problem. Finally, \(\lim v_{i+1} = -\lim \nabla F^0_i(x_i) = -\nabla F^0_i(z) = v_{\text{KS}}\) is the KS potential. \(\square\)

As noted above, the reference system reproduces the quasi-density \(z\) of the full system and they link back to the real densities by (10),
\[
\rho = z + \varepsilon v, \quad \rho_{\text{KS}} = z + \varepsilon v_{\text{KS}}, \tag{27}
\]
where typically $\rho_{KS} \neq \rho$. Then $v_{KS} - v = e^{-1}(\rho_{KS} - \rho)$ is precisely the Hxc potential that depends on the regularization parameter $\varepsilon$ here. This means every choice of $\varepsilon$ defines a different reference system. A limit $\varepsilon \to 0$ in the algorithm is unfeasible because of its relation to the step length.

A simulation of two electrons in a discretized one-dimensional quantum ring \cite{22} allows us to illustrate the above method numerically. A previously reported implementation of MYKSODA-L in a CDFT setting \cite{18} has been adapted to a pure DFT setting and extended by MYKSODA-S. A radius of $R = 1$ bohr, a uniform grid with 30 points, and the interaction energy $H_{int} = 3\sqrt{1 + \cos(\theta_1 - \theta_2)}$ were used in the reported example. As expected, larger $\varepsilon$ leads to faster convergence. Also, the more conservative steps taken by MYKSODA-S often lead to slower convergence in practice. Surprisingly, however, in some cases MYKSODA-S overtakes the less conservative MYKSODA-L. An example is shown in Fig. 3. Such a crossover is possible as the two algorithms follow different paths through the space of densities and potentials. Yet when the starting point is the same, the first step by MYKSODA-L always lowers the energy more than the first step by MYKSODA-S. Although it is a plausible conjecture that also MYKSODA-L, taking maximal steps, is guaranteed to converge, the present proof does not establish this. Maximal steps here mean taking $\tau_1$ maximally such that $\langle \nabla F_\varepsilon(x_{i+1}) + v, x_{i+1} - x_i \rangle \leq 0$ which means maximal decrease in energy in the direction chosen by step (b).

In this letter we proved convergence of the exact, regularized Kohn–Sham iteration scheme with special adaptive damping. In short this means that KS-DFT is a veritable method to calculate the correct ground-state density. This strong statement holds for all flavors of DFT that are defined on a finite-dimensional density space $X = L^2(M)$ and have a linear coupling to external potentials of type $\langle v, \rho \rangle$. This includes CDFT, where the potential $v$ is a combination of scalar and vector potential, and the density $\rho$ includes the paramagnetic current density. To allow for a combination of these different entities into one Banach space setting, the respective function spaces for one-particle densities and current densities have to fulfill a condition termed “compatibility” in Laestadius et al. \cite{13}. A proof of MYKSODA convergence for infinite-dimensional Banach spaces $X$ is feasible too, but turns out to be much more technical and will be presented elsewhere. The choice of step length implemented in (c) here is an essential part of the proof and similar choices could be of value in showing convergence of other ODA iteration schemes like for Hartree–Fock \cite{10}. Next to this damping step the MY regularization is a vital part of the proof at hand, not only to have functional differentiability, but also for the strong monotonicity estimate needed to show convergence. How these findings can be transferred to realistic KS implementations will be the content of future research, but it is expected that they serve as useful guidelines for better convergence results.

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