Exact Kohn-Sham Density Functional Theory on a Lattice

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Abstract

We formulate a set of equations that facilitate an exact numerical solution of the Kohn-Sham potential for a finite Hubbard chain with nearest neighbour hopping and arbitrary site potentials. The approach relies on a mapping of the non-interacting Kohn-Sham ground state wave function onto the exact interacting system wavefunction and two interconnected self-consistent cycles. The self-consistent cycles are performed within the framework of the Kohn-Sham non-interacting system without any direct reference to the interacting system. The first self-consistent cycle updates the mapping of the non-interacting wavefunction onto the interacting wavefunction based on a trial input density, while the second self-consistent cycle updates the Kohn-Sham potential to yield the trial density. At the solution point, the exact density, the exact Kohn-Sham potential, the density functional correlation energy and the exact interacting system ground state energy are available.

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Density Functional Theory (DFT) on a Lattice (L-DFT) has a history that dates back to its introduction by Schönhammer and Gunnarson in 1987. It is also called a Site Occupation Number Function Theory (SOFT) since on a lattice, DFT is formulated in terms of the site occupation numbers, based on the Hohenberg-Kohn theorem that the ground state density is the controlling variable which determines all the properties of the system. Kohn and Sham suggested an implementation of DFT where the interacting systems is mapped onto a fictitious non-interacting system that yields the same density as the interacting system. It is the Kohn-Sham (KS) implementation of DFT that has lead to the popularity of DFT. The fundamental principles on which DFT relies can be applied to any many-particle Hamiltonian. Here we are interested in one dimensional Hubbard Hamiltonian. Despite its simplicity, the Hubbard model has been extremely successful in developing an understanding of highly correlated many-particle systems. However, when inhomogeneities are introduced, even simple lattice models quickly become numerically intractable. Here L-DFT can play an important role. Some of the attractions of L-DFT is the simplicity of the model, the known solution of the infinite uniform system and the possibility to solve the model for short finite chains exactly. L-DFT has been used to explore formal properties of exact functionals. The model provides an ideal environment for studying formal properties since it is possible to determine exact properties, which is informative on their own, but it also provides a reference to which approximations can be compared.

In this paper we present an exciting development for L-DFT. We have formulated a set of equations that can be used iteratively to solve the L-DFT problem for a finite chain exactly. Consider a finite one dimensional single band interacting Hubbard Hamiltonian with nearest neighbour hopping.

\[
\hat{H} = -t \sum_{<i,j>,\sigma} \hat{c}_{j\sigma}^\dagger \hat{c}_{i\sigma} + U \sum_{i} \hat{n}_{i\uparrow} \hat{n}_{i\downarrow} + \sum_{i,\sigma} v_{i} \hat{n}_{i\sigma},
\]

(1)

where \( \hat{c}_{i\sigma}^\dagger \) and \( \hat{c}_{i\sigma} \) are the creation and annihilation operators of an electron with spin \( \sigma \) in the localised state at site \( i \), respectively. The summation \( <i,j> \) is over nearest neighbours only and we consider a finite system. \( \hat{n}_{i\uparrow} = \hat{c}_{i\uparrow}^\dagger \hat{c}_{i\uparrow} \) is the site occupation number operator for spin \( \sigma \), while \( v_{i} \) is a site potential and \( U \) is the on-site interaction strength. We choose the hopping strength \( t > 0 \). The eigenspectrum of \( \hat{H} \) is invariant under a change of the sign of
but the eigenfunctions are not. The total spin operator $\sum_{i=1}^{N} \hat{n}_{i\sigma}$ commutes with the Hamiltonian,
\[
\left[ \sum_{i=1}^{N} \hat{n}_{i\sigma}, \hat{H} \right] = 0,
\]
and therefore the numbers of up-spin, $N$, and down-spin, $N_{\downarrow}$, electrons are good quantum numbers. We are interested in the lowest energy solutions of the Schrödinger equation under the constraint of a fixed number of up- and down-spin electrons,
\[
\hat{H} |\Psi(N_{\uparrow}, N_{\downarrow})\rangle = E |\Psi(N_{\uparrow}, N_{\downarrow})\rangle.
\]
As a consequence the spin constrained ground states of $\hat{H}$ can be expended in terms of Slater determinants $|\phi_{m}\rangle$ with the same spin constraint as the ground state. The subscript $m \equiv \{N_{\uparrow}, N_{\downarrow}, N_{L}\}$ is a compound index which represents all possible basis functions for a chosen spin polarisation, $N_{\uparrow}$, $N_{\downarrow}$, and number of sites, $N_{L}$. We follow the notation of Lieb and Wu and label the lattice sites sequentially from the left. The basis functions $|\phi_{m}\rangle$ can be represented by an $n_{e}$-tuple ($n_{e} = N_{\uparrow} + N_{\downarrow}$)
\[
|\phi_{m}\rangle = \hat{c}_{x_{1}^{m}}^\dagger \hat{c}_{x_{2}^{m}}^\dagger \cdots \hat{c}_{x_{N_{\uparrow}}^{m}}^\dagger \hat{c}_{x_{N_{\uparrow}+1}^{m}}^\dagger \hat{c}_{x_{N_{\uparrow}+2}^{m}}^\dagger \cdots \hat{c}_{x_{n_{e}}^{m}}^\dagger)
\]
\[
\equiv (x_{1}^{m}, x_{2}^{m}, ..., x_{n_{e}}^{m})
\]
where the first $N_{\uparrow}$ entries, $x_{i}^{m}$, $x_{i}^{m} < x_{i+1}^{m}$, label the sites $x_{i}^{m}$ in the Slater determinant with $|\phi_{m}\rangle$ with occupied up-spin states and the $N_{\uparrow} + 1$ to $n_{e}$ entries, $x_{i}^{m} < x_{i+1}^{m}$, label the sites where localised down-spin states are occupied. The states $|\Psi(N_{\uparrow}, N_{\downarrow}, v)\rangle$ can be expanded in terms of the corresponding spin constrained basis functions as
\[
|\Psi(N_{\uparrow}, N_{\downarrow}, v)\rangle = \sum_{m} f_{m} |\phi_{m}\rangle.
\]
The lattice non-interacting Hamiltonian $\hat{H}^{0}$ is defined as
\[
\hat{H}^{0}(v^{0}) = -t \sum_{<i,j>, \sigma} \hat{c}_{i\sigma}^\dagger \hat{c}_{j\sigma} + \sum_{i, \sigma} v_{i}^{0} \hat{n}_{i\sigma},
\]
with ground state solutions
\[
|\Phi(N_{\uparrow}, N_{\downarrow}, v^{0})\rangle = \sum_{m} g_{m} |\phi_{m}\rangle.
\]
When the site potential $v^{0}$ is equal the Kohn-Sham site potential, $v^{KS}$, the interacting and non-interacting site densities, $n_{i}$, are identical,
\[
n_{i} = \langle \Psi | \hat{n}_{i\uparrow} + \hat{n}_{i\downarrow} | \Psi \rangle = \langle \Phi | \hat{n}_{i\uparrow} + \hat{n}_{i\downarrow} | \Phi \rangle
\]
For ease of notation, we have suppressed the total spin and potential in the notation of the wave functions.

We partition the interacting system energy as

$$E = \langle \Psi \left| \hat{H} \right| \Psi \rangle = T^{KS} + E^{hx} + E^c + \langle \Phi \left| \hat{v} \right| \Phi \rangle \tag{9}$$

where

$$T^{KS} = \langle \Phi \left| \hat{T} \right| \Phi \rangle$$

$$E^{hx} = \langle \Phi \left| \hat{u} \right| \Phi \rangle$$

$$E^c = \langle \Psi \left| \hat{T} + \hat{u} \right| \Psi \rangle - \langle \Phi \left| \hat{T} + \hat{u} \right| \Phi \rangle$$

$$\langle \Phi \left| \hat{v} \right| \Phi \rangle = \langle \Psi \left| \hat{v} \right| \Psi \rangle = \sum_i v_i n_i \tag{10}$$

$E^c$ is has the form of the conventional correlation energy while $E^{hx}$ is the sum of the equivalent conventional Hartree and exchange energies. The ground state energies are functions of the site densities and the requirement that the ground state site densities of the interacting and non-interacting systems are identical requires that

$$v_i^{KS} = v_i + \frac{d}{dn_i} \left( E^{hx} + E^c \right). \tag{11}$$

The $hx$ term in Eq. (10), by definition, depends on the Kohn-Sham (KS) ground state wavefunction only. When the correlation is set to zero, the KS equation can be solved self-consistently without further approximation. The correlation term, on the other hand, depends on the interacting and non-interacting system ground state wavefunctions and is the term that has proven to be the most challenging to approximate. Here we follow a different approach and formulate an expression for the correlation energy that can be solved within a non-interacting framework without any direct reference to the interacting system.

The interacting and non-interacting wavefunctions can be expanded in terms of the same basis functions and we map the non-interacting wave function onto the interacting wavefunction

$$|\Psi\rangle = \hat{J} |\Phi\rangle. \tag{12}$$

with

$$\hat{J} = \sum_m e^{-\gamma_m} \hat{x}^m \tag{13}$$
where the projection operator \( \hat{x}^m = \hat{x}_1^m \cdots \hat{x}_n^m \). The \( \hat{x}_i \) are equal to \( \hat{n}_{x_i \uparrow} \) if \( i \leq N \uparrow \) and \( \hat{n}_{x_i \downarrow} \) otherwise. The expansion coefficients in Eqs. (5) and (7) are simply related,

\[
f_m = e^{-\gamma_m} g_m.
\]  

(14)

We can work in real space without losing generality. For the single band linear Hubbard model with nearest neighbour mapping, the ground state wavefunction is non-degenerate and for \( t > 0 \), the expansion coefficients \( f_m \) and \( g_m \) are non-zero and all have the same sign. It follows that when the \( f_m \) and \( g_m \) are chosen to have the same sign, the mapping in Eq. (14) is well defined. The operator \( \hat{J} \) commutes with \( \hat{u} \) and \( \hat{v} \) and we can write

\[
\left( \hat{J}^{-1} \hat{T} \hat{J} + \hat{u} + \hat{v} \right) |\Phi\rangle = E |\Phi\rangle
\]  

(15)

where \( E \) is the ground state energy of the interacting system. Taking the expectation value with respect to \( |\Phi\rangle \), and assuming that all wavefunctions are normalised, the interacting system energy can be expressed as

\[
\langle \Phi | \hat{J}^{-1} \hat{T} \hat{J} + \hat{u} + \hat{v} |\Phi\rangle = E.
\]  

(16)

Knowledge of \( \hat{J} \) is then sufficient to find the interacting energy with reference to the non-interacting system ground state wavefunction only.

We have

\[
\langle \phi_m | \hat{J}^{-1} \hat{T} \hat{J} |\Phi\rangle = -t \sum_{i=1}^{n_e} \sum_{s=\pm1} g(x^m_{i | x^m_{i + s} | e^{-\gamma_m | x^m_{i + s} |}}) e^{\gamma_m}
\]  

(17)

where \( x^m_{i | x^m_{i + s} |} \) represents the \( n_e \)-tuple with the occupancy of site \( x^m_{i} \) decreased by one and the occupancy of a neighbouring site (+ to the right and - to the left) increased by one. If this results in a double occupancy of the same spin or if a non-existing site of the finite chain is occupied, the resulting coefficient \( g(x^m_{i | x^m_{i + s} |}) = 0 \). From Eq. (10) the correlation energy can be written as

\[
E^c = \langle \Phi | \hat{J}^{-1} \hat{T} \hat{J} - \hat{\mathcal{T}} |\Phi\rangle
\]  

\[
= -t \sum_{m,m'} g(x^m) \sum_{i=1}^{n_e} \sum_{s=\pm1} g((x^m_{i | x^m_{i + s} |}) \equiv x^m_{i}) (e^{-\gamma_m | x^m_{i + s} |} e^{\gamma_m} - 1),
\]  

(18)

and from Eqs. (16) and (17) we get

\[
e^{\gamma_m} = \frac{g(x^m) \langle \phi_m | (E - \hat{u} - \hat{v}) |\phi_m\rangle}{-t \sum_{i=1}^{n_e} \sum_{s=\pm1} g(x^m_{i | x^m_{i + s} |}) e^{-\gamma_m | x^m_{i + s} |}}.
\]  

(19)
The expressions in Eqs. (18) and (19) are correct at the solution point only. The site densities for the interacting, \( n_i \), and non-interacting, \( n_i^0 \), systems can be expressed as

\[
n_i = \sum_m e^{-2\gamma_m} g^2 (x^m) \langle x^m | \hat{n}_{i\uparrow} + \hat{n}_{i\downarrow} | x^m \rangle
\]

and

\[
n_i^0 = \sum_n g^2 (x^m) \langle x^m | \hat{n}_{i\uparrow} + \hat{n}_{i\downarrow} | x^m \rangle.
\]

In the Kohn-Sham formalism, the site densities of the interacting and fictitious KS-system must be identical, \( n_i = n_i^0 \), and this is key to the solution outlined below. It is possible to derive expressions for the Kohn-Sham site potentials \( v_i + \frac{d}{dn_i} (E^{hx} + E^c) \) using the site analogue of the outline given in [19, 20], but \( E \) and \( |\Psi\rangle = \hat{J} |\Phi\rangle \) can be found without knowledge of \( \frac{d}{dn_i} (E^{hx} + E^c) \) by directly determining \( v_i^{KS} \) iteratively in a double self-consistent calculation as follows:

Approximate \( v_i^0 \) and find the ground state wavefunction for the corresponding non-interacting Hamiltonian \( H^0 \), of Eq. (6). Choose an initial set of parameters \( \{\gamma_m\} \). Repeat the following self-consistent cycles till self consistency is reached:

1. Use Eq. (16) to approximate \( E \{\gamma_m\} \). Iterate Eq. (19) for \( \{\gamma_m\} \) to a self-consistent solution for the fixed input \( g(x^m) \) from the solution of \( H^0 \).

2. Determine \( n_i \{\gamma_m\} \) from previous solution of \( g(x^m) \) and \( \{\gamma_m\} \) from cycle 1. Keep \( n_i \{\gamma_m\} \) fixed and update \( v_i^0 \) till \( n_i^0 [v^0] = n_i \{\gamma_m\} \). Use the output \( g(x^m) \) and repeat cycle 1.

When the two cycles reach self-consistency simultaneously, we have a solution where the interacting and non-interacting densities are identical. This is simply the requirement for, or definition of, the KS fictitious system, the non-interacting system that gives the same density as the fully interacting system [6]. Therefore, at self-consistency, \( v^0 = v^{KS} \). Note that if Eq. (19) is satisfied, the energy \( E \{\gamma_m\} \) is the variationally minimised energy of \( H \) under the constraint that the expansion coefficients \( e^{-\gamma_m} g(x^m) \) all have the same sign. Since we use a complete basis set for each spin polarisation, \( E \{\gamma_m\} \) is the interacting ground state energy for the corresponding spin polarisation. In this approach we not only get the exact KS-lattice potential, but also the exact interacting particle wave function.
If is a simple matter to perform the diagonalisation of the KS-system by determining the eigensolutions of a single particle Hamiltonian and then expand the many-particle ground state wavefunction in terms of the many-particle basis functions introduced above. This makes the approach flexible and allows solution for long finite chains.

In our tests for Hubbard chains up to 10 sites long, a simple self-consistent iteration cycle, where a fraction of the output of a cycle, \( \{\gamma_m\} \) or \( \{v^0_i\} \), is added to the corresponding value of the previous cycle, scaled by an appropriate factor, always converged to the exact value.

In conclusion, we have formulated a set of equations that allows us to solve the Kohn-Sham equations exactly for a finite Hubbard chain with nearest neighbour hopping. The approach relies on the unique property of the model that the expansion coefficients of the ground state wavefunction in terms of an appropriate set of Slater determinant basis functions have the same sign. The ideas introduced may, however, have potential in a more general setting.

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