Simple parameterization for the ground-state energy of the infinite Hubbard chain incorporating Mott physics, spin-dependent phenomena and spatial inhomogeneity

Vivian V França¹,²,⁵, Daniel Vieira³ and Klaus Capelle⁴

¹ Physikalisches Institut, Albert Ludwigs Universität, Hermann-Herder 3, 79104 Freiburg, Germany
² Capes Foundation, Ministry of Education of Brazil, Caixa Postal 250, Brasilia 70040-20, Brazil
³ Departamento de Física, Universidade do Estado de Santa Catarina, Joinville, 89219-710 SC, Brazil
⁴ Centro de Ciências Naturais e Humanas, Universidade Federal do ABC (UFABC), Santo André, 09210-170 SP, Brazil
E-mail: vivian.franca@physik.uni-freiburg.de

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Abstract. Simple analytical parameterizations for the ground-state energy of the one-dimensional repulsive Hubbard model are developed. The charge dependence of energy is parameterized using exact results extracted from the Bethe-ansatz (BA). The resulting parameterization is shown to be in better agreement with highly precise data obtained from a fully numerical solution to the BA equations than previous expressions (Lima et al 2003 Phys. Rev. Lett. 90 146402). Unlike these earlier proposals, the present parameterization correctly predicts a positive Mott gap at half filling for any $U > 0$. The construction is extended to spin-dependent phenomena by parameterizing the magnetization dependence of the ground-state energy using further exact results and numerical benchmarking. Lastly, the parameterizations developed for the spatially uniform model are extended by means of a simple local-density-type approximation to spatially inhomogeneous models, e.g. in the presence of impurities, external

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5 Author to whom any correspondence should be addressed.
fields or trapping potentials. The results are shown to be in excellent agreement with independent many-body calculations, at a fraction of the computational cost.

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1. Introduction

The Mott insulator is the archetypal strong-correlation phenomenon [1]. It is well known that in a first-principles description of such systems by means of density-functional theory (DFT) one encounters considerable difficulty. The single-particle (Kohn–Sham (KS)) gap calculated with standard DFT methodology is not the same as the many-body gap, even in principle and even if no approximations are made during the calculation. In the particular case of the Mott insulator, it is known that a proper description of the Mott gap is obtained by adding to the single-particle KS gap a correction arising from the derivative discontinuity of the exchange-correlation functional [2–7].

Many modern density functionals have an implicit derivative discontinuity due to their orbital dependence, but this affords at best an incomplete description of the Mott state and the Mott gap [3, 6, 7]. Only a very few density functionals have an explicit discontinuity as a function of the density, including the two-electron functional of Mori-Sanchez et al [3], which is based on the so-called flat-plane condition devised by the same authors [3–5], and the Bethe-ansatz local-density-type approximation (BALDA) of Lima et al [8, 9], which is based on an approximate analytical parameterization of the Bethe-ansatz (BA) solution for the ground-state energy of the one-dimensional Hubbard model (1DHM) that becomes exact in several important limits. Both of these functionals properly account for the Mott insulator. Only the BALDA, however, has been parameterized in a way that allows its application to a wide range of physical systems. As a consequence, BALDA and variations thereof have been applied to inhomogeneous correlated many-electron systems as well as to correlated many-atom systems in optical lattices and traps [9–18].

However, in these applications it has become clear that the parameterization by Lima et al., also referred to as LSOC parameterization after the initials of its developers, still does not provide a fully correct description of the Mott gap. In particular, at small $U$ the LSOC expression for $E_c$ has a derivative discontinuity, but the resulting Mott gap is negative, effectively predicting the Mott state to be a (strange) metal instead of an insulator. It is not trivial to correct this behaviour, as any change to the LSOC expression must preserve the exact limits and properties already built into it. Thus, instead of merely algebraic adjustments, it becomes necessary to understand and improve the physics missing from the LSOC parameterization in this regime.
A key aspect of the Mott insulator is that it is a nonmagnetic state of matter, i.e. the insulating nature is not the result of antiferromagnetism. Therefore, the solution to the problem just described must be expressed, within DFT, in terms of charge density only, and cannot make use of spin densities and spin-density-functional theory (SDFT). On the other hand, many correlated systems do have magnetic phases. Therefore, a more complete description of strong correlations must properly account for both, the insulating state and various types of magnetic states, as well as their possible coexistence. While such a description is possible within BA-based SDFT by performing a fully numerical (FN) solution to the spin-resolved BA equations and interpolating between the resulting data points every time the exchange-correlation energy needs to be evaluated, this procedure is very inconvenient for KS calculations, where the functional must be evaluated hundreds or thousands of times during the iterations towards self-consistency. A simple parameterization of the spin dependence would allow straightforward application of BA-DFT methodology to spin-dependent phenomena in electronic systems and hyperfine-label-dependent phenomena in optical lattices.

This paper reports the progress made along both of these lines. In section 2, we identify a shortcoming of the standard parameterization used in BALDA and propose a simple, ad hoc but physically motivated, variation of it that is more accurate and whose Mott gap properly remains positive for all values of the interaction $U$. The revised parameterization also considerably improves the description of the metallic (e.g. Luttinger liquid) phases. In section 3, we employ exact analytical results extracted from the BA to further generalize this revised parameterization to spin-dependent situations. In section 4, we use a simple local-density-type approximation to extend our results to spatially nonuniform systems. Density-matrix renormalization group (DMRG) and Lanczos calculations are performed to test and validate this approximation. Section 5 gives a brief summary.

2. Improved description of the Mott gap

The task at hand is to obtain a simple and accurate analytical approximation for the ground-state energy $E_0$ of the inhomogeneous 1DHM,

$$\hat{H} = -t \sum_{i,\sigma} (\hat{c}_{i\sigma}^\dagger \hat{c}_{i+1,\sigma} + \text{h.c.}) + U \sum_i \hat{n}_{i\uparrow} \hat{n}_{i\downarrow} + \sum_{i,\sigma} V_i \hat{n}_{i\sigma},$$

where $\hat{n}_{i\sigma} = \hat{c}_{i\sigma}^\dagger \hat{c}_{i\sigma}$ is the spin-resolved particle-density operator at site $i$, $\hat{c}_{i\sigma}$ and $\hat{c}_{i\sigma}^\dagger$ are fermionic creation and annihilation operators, $t$ is the hopping parameter (taken to be the unit of energy), $U$ is the on-site interaction and $V_i$ is an on-site potential that makes the system spatially inhomogeneous. In applications to electrons in crystal lattices, $V_i$ can describe inequivalent atoms in the lattice, while in applications to cold atoms in optical lattices it accounts for the trapping potential.

The commonly used expression for the per-site ground-state energy ($e_0$) of the 1DHM is the LSOC parameterization, given by [8]

$$e_0^{\text{LSOC}}(n, U) = -\frac{2\beta(U)}{\pi} \sin \left( \frac{\pi n}{\beta(U)} \right),$$

where $\beta(U) = \sqrt{U^2 - 4t^2}$ is the Fermi level for a uniform system.
where \( n = n_+ + n_- \) is the charge density and the interaction \( U \) enters \( e_0(n, U) \) through the interaction function \( \beta(U) \), which is determined from

\[
-\frac{2\beta(U)}{\pi} \sin \left( \frac{\pi}{\beta(U)} \right) = -4 \int_0^{\infty} \frac{J_0(x)J_1(x)}{x \left( 1 + e^{Ux/2} \right)} dx. \tag{3}
\]

By construction, this expression becomes exact for \( U \to 0 \) and any \( n \) (where \( \beta = 2 \)), for \( U \to \infty \) and any \( n \) (where \( \beta = 1 \)), and for \( n = 1 \) and any \( U \) (where \( 0 \leq \beta \leq 1 \)), and provides a reasonable approximation to the full BA solution in between.

In the LSOC parameterization, the interaction function \( \beta(U) \) is independent of the particle density and of spin. This independence is algebraically very convenient, as it allows one to determine \( \beta(U) \) outside the self-consistency cycle of DFT instead of having to recalculate it any time the charge (or spin) density changes. However, it is physically incorrect, as the relation between the bare interaction parameter \( U \) and the correlation energy \( E_c \) must depend on the charge density, e.g. through screening. As a consequence of the density independence of \( \beta \), LSOC retains the sinusoidal density-dependence of the energy, which is correct only at \( U = 0 \) and \( U \to \infty \), also for all intermediate values of \( U \).

Thus, it becomes necessary to modify the interaction function in a way that allows it to change with the density. The additional density dependence, however, must not spoil the behaviour in the three limits exactly recovered by LSOC. This condition severely restricts the modifications that could possibly be made to the LSOC parameterization. The form we adopt is

\[
e_0^{FVC}(n, U) = -\frac{2\beta(n, U)}{\pi} \sin \left( \frac{\pi n}{\beta(n, U)} \right), \tag{4}
\]

where \( \beta(n, U) = \beta(U)^{\alpha(n, U)} \) and \( \alpha(n, U) = n^{\sqrt{U/8}} \). We stress that this particular form has not been derived from first principles but is a physically motivated ad hoc modification designed to restore the density dependence of the interaction function through the replacement \( \beta(U) \to \beta(n, U) \), while preserving all exact limits obeyed by the LSOC expression. The specific form chosen for the exponent \( \alpha(n, U) \) is a consequence of the later generalization to spin-dependent phenomena, as explained in section 3.

Figure 1 compares the present parameterization (4) to the data obtained from an FN solution to the BA integral equations. For comparison purposes, the earlier LSOC parameterization (2) is also included. To distinguish the present from the LSOC expression, we label the curves corresponding to the former by FVC. As the insets show, the relative deviation of FVC data from FN data is typically less than 2% and at most \(~4\%\). This is the same size of error of the LDA itself (quantified by comparing the BALDA/FN data for small Hubbard chains to the results from exact diagonalization), so that to within the accuracy of the LDA the present parameterization is a faithful representation of the full BA solution for the entire parameter range, including values of \( U \gg 6t \) that cannot be realized in solids but occur in systems of trapped cold atoms.

Our main motivation for developing equation (4), however, was the incorrectly negative Mott gap predicted by the LSOC expression between \( U = 0 \) and \( U = 2t \). The Mott gap \( E_{\text{gap}} \) can analytically be evaluated from the expression for \( e_0(n, U) \), either by explicitly calculating the derivative discontinuity or by taking total energy differences [9]. From the LSOC
parameterization, one obtains [9]

\[ E_{\text{LSOC}}^{\text{gap}}(U) = U + 4 \cos \left( \frac{\pi}{\beta(U)} \right) \]  

(5)

whereas the present parameterization leads to

\[ E_{\text{FVC}}^{\text{gap}}(U) = U + 4 \cos \left( \frac{\pi}{\beta(U)} \right) - \frac{1}{2} \beta(U) U^{1/3} \ln \beta(U) \]

\[ \times \left[ -\frac{1}{\pi} \sin \left( \frac{\pi}{\beta(U)} \right) + \frac{1}{\beta(U)} \cos \left( \frac{\pi}{\beta(U)} \right) \right]. \]  

(6)

As illustrated in figure 2, additional terms arising from the present expression push the gap upward, avoiding it becoming negative between \( U = 0 \) and \( U = 2t \) as was incorrectly the case within the LSOC expression [9]. For \( U > 2t \) both the LSOC and the present (FVC) gap are positive, the latter being significantly closer to the numerical BA results than the former, although neither reproduces the subtle nonperturbative behaviour for \( U \to 0 \), in spite of the logarithmic term in equation (6). Only within the latter, however, the Mott gap is everywhere positive.

3. Extension to spin-dependent phenomena

In spin-polarized situations, the energy depends on the spin density \( m = n_\uparrow - n_\downarrow \), in addition to the charge density \( n = n_\uparrow + n_\downarrow \) and the interaction \( U \). This dependence is not included in the LSOC parameterization, which therefore cannot be applied to study spin-dependent phenomena for electrons in solids or hyperfine-polarization-dependent phenomena for atoms in optical lattices. We note that Bethe-ansatz local-spin-density approximation (BALSDA) calculations for the 1DHM have already been performed in the context of cold atoms in optical lattices [19–21]. In lieu of an analytical parameterization, these works resorted to an FN solution.
of the BA integral equations. An analytical parameterization would substantially simplify this approach, making the BALSDA as easily implementable as the BALDA one.

An additional advantage of the analytical approach over the numerical one is that in the solution to the BA integral equations one cannot specify from the outset the density and magnetization of the system one is interested in. Rather, one has to specify the upper and lower limits of the integrals, and obtain the densities as part of the solution. This is clearly inconvenient for DFT, where the energies have to be evaluated as functions of the densities. More generally, it is desirable to be able to specify the system under study in terms of physical observables, such as the densities $n$ and $m$, instead of in terms of auxiliary quantities, as the limits of the BA integrals.

Analytical expressions also permit one to derive further analytical results for other quantities. Our present derivation of closed expressions for the Mott gap is one example, and the analytical derivation and solution of Euler equations determining the phase diagram of harmonically trapped fermions on optical lattices [17] is another. For all these reasons, a simple but reliable parameterization of $e_0(n, m, U)$ can be useful for various types of calculations, within SDFT and beyond. Therefore, we next present an analytical parameterization of $e_0(n, m, U)$ and use it to construct a BALSDA for the 1DHM.

In order to generalize the LSOC and FVC expressions to spin-dependent situations, we once more follow the basic philosophy of constructing an analytical interpolation function recovering exactly known limits as a function of the physically relevant variables. Several such exact results for $e_0(n, m, U)$ are known [22–24]. For noninteracting systems ($U = 0$),

$$e_0(n, m, U = 0) = -\frac{4}{\pi} \sin\left(\frac{\pi n}{2}\right) \cos\left(\frac{\pi m}{2}\right).$$

(7)

For infinite interaction ($U \to \infty$),

$$e_0(n, m, U \to \infty) = -\frac{2}{\pi} \sin(\pi n).$$

(8)
For half-filled unpolarized systems \((n = 1, m = 0)\),

\[
e_0(n = 1, m = 0, U) = -4 \int_0^\infty dx \frac{J_0(x) J_1(x)}{x \left(1 + \exp^{Ux/2}\right)}.
\] (9)

Finally, for maximum magnetization \((m = n)\),

\[
e_0(n, m = n, U) = -\frac{2}{\pi} \sin(\pi n).
\] (10)

The LSOC and FVC parameterizations take \(m = 0\), and express \(e(n, U)\) as a controlled analytical interpolation between (8) and (9) and the \(m = 0\) limit of (7). The construction of a more complete interpolation, recovering all four limits as functions of \(n, m\) and \(U\), is strongly constrained by these limits, but still not unique. We therefore impose five additional common-sense criteria: (i) avoid high-order polynomials, which can produce unphysical wiggles; (ii) avoid unusual special functions; and (iii) keep the form similar to the LSOC parameterization. This third condition is useful because the LSOC parameterization has now been implemented and used by many groups \([9–14]\), so it will be easier to update to a new parameterization which has a similar form to the old one. However, as we have argued above, the LSOC expression does not properly describe the density dependence of the ground-state energy at intermediate \(U\). Therefore, we also require, as condition (iv), that our spin-dependent generalization reduce to the present equation (4) for \(m = 0\) instead of to equation (2). The final, fifth, additional condition is motivated by computational efficiency and is explained in section 4. Even with these additional common-sense criteria, the form of the parameterization is not uniquely determined, and a very large function space can still be explored. The particular choice made below was obtained by starting from the LSOC form and then building in, one by one, additional exact limits and criteria. Many different variations have been explored, but we stopped when arriving at one whose deviation from the FN solution to the BA equations was less than the typical error bar of the LDA for this type of system. At this point, further improvements in the form of the parameterization become indistinguishable, in applications to inhomogeneous systems, from the intrinsic error of the LDA.

All four exact limits and five supplementary conditions are incorporated by the choice

\[
e_{0}^{\text{FVC}}(n, m, U) = -\frac{2\beta(n, m, U)}{\pi} \sin \left(\frac{\pi n}{\beta(n, m, U)}\right) \cos \left(\frac{\pi m}{\gamma(n, m, U)}\right),
\] (11)

where

\[
\beta(n, m, U) = \beta(U)^{\alpha(n, m, U)},
\] (12)

\[
\gamma(n, m, U) = 2 \exp \left[\frac{\sqrt{U}}{1 - (m/n)^{3/2}}\right],
\] (13)

and

\[
\alpha(n, m, U) = \left[\frac{n^2 - m^2}{n^{15/8}}\right]^{3/8} \sqrt{U}.
\] (14)

Here, \(\beta(U)\) is the same quantity employed in the LSOC parameterization. For zero magnetization, \(\alpha(n, m, U)\) reduces to \(\alpha(n, U)\) used in equation (4). Equation (11) is valid...
Figure 3. Per-site ground-state energy as a function of magnetization, for $n \sim 0.5$ and several values of $U$. Inset: percentage deviation from the FN data, defined as $100(e_{\text{FVC}}(\text{LSOC}) - e_{\text{FN}})/e_{\text{FN}}$.

for $U \geq 0$ and $n \leq 1$, but it can be extended to $n > 1$ and to $U < 0$ by standard particle–hole transformations [9, 17, 22, 24].

Satisfaction of condition (10) is of particular interest because this condition has no counterpart in the spin-independent situation. Moreover, it establishes a coupling between the charge and the spin dependence. Physically, maximum spin means that the Pauli principle keeps all fermions maximally apart for any $U$, just as infinitely repulsive interactions ($U \to \infty$) do for any degree of spin polarization. For $n = m$ the spin-dependent parameterization must thus reduce to the same limit as for $U \to \infty$ and recover the value $\beta = 1$. On the other hand, for $m = 0$ the expression should reduce to the earlier form (4). This double requirement is the explanation of the particular form chosen for $\alpha(n, m, U)$ of equation (14) and, consequently, for $\alpha(n, U)$ of equation (4).

Figure 3 presents a comparison of the spin dependence of this parameterization with the data obtained from an FN solution to the BA integral equations for intermediate parameter values, where the expression is not exact already by construction. Clearly, the spin dependence of the homogeneous system is recovered to within the same precision as the charge dependence.

4. Local approximation for inhomogeneous systems

The main use of DFT and SDFT is in calculations for spatially inhomogeneous systems, where translational symmetry is broken and the density becomes position dependent. In the case of lattice models, inhomogeneity means that not all sites are equivalent. By means of the L(S)DA prescription, expressions for the energy of the homogeneous system, such as those described in the preceding section, can be used on a site-by-site basis to approximate the corresponding energy of the inhomogeneous system.
Explicitly, the LSDA to any energy component $E$ is given by

$$ E \approx E^{\text{LSDA}} = \sum_{i} e(n, m, U)|_{n \to n_i, m \to m_i}, $$

(15)

where $L$ is the number of lattice sites, and $e = \lim_{L \to \infty} E(L)/L$ is the per-site energy of the homogeneous system. This expression approximates the energy of the inhomogeneous system, where $n_i$ and $m_i$ vary from site to site, by evaluating the energy density of the homogeneous system site by site at the densities of the inhomogeneous one. In DFT, including model DFT, this prescription is usually applied to the correlation energy, which for the Hubbard model can be defined as $E_c = E_0 - E_{\text{MF}}$, where $E_{\text{MF}}$ is the mean-field approximation to the ground-state energy $E_0$. Since $E_{\text{MF}}$ is simple to obtain, the task to approximate the correlation energy $E_c[n_i, m_i, U]$ of the inhomogeneous Hubbard model is thus reduced to that of approximating the per-site ground-state energy of the homogeneous one, $e_0(n, m, U)$. This is the quantity that we extracted above from the BA equations.

The minimization of the resulting energy functional is conveniently carried out via self-consistent KS calculations of the charge and spin densities and of the resulting ground-state energies. In such KS calculations the correlation potentials (obtained by differentiating the correlation energy with respect to $n$ and $m$ or, equivalently, to $n_\uparrow$ and $n_\downarrow$) are evaluated once in each of the iterations of the self-consistency cycle. In these iterations, the densities $n_i$ and $m_i$ change, but the interaction $U$, being a parameter of the Hamiltonian, does not. We have therefore expressed the integral in equation (3) and the resulting transcendental equation for $\beta$ exclusively in terms of $U$, in order to guarantee that the slightly time-consuming steps of the calculation take place only once in each calculation, outside the self-consistency cycle. This is the fifth additional condition on the spin-dependent parameterization alluded to above.

As a simple example of such KS calculations, which serves to illustrate all essential aspects, we consider open Hubbard chains, where the spatial inhomogeneity stems from the boundaries, which give rise to charge and spin-density oscillations in the bulk. Representative results for a chain with $L = 100$ sites are displayed in figure 4, where we compare the ground-state density profile (figure 4(a)) and spin-density profile (figure 4(b)) obtained DMRG to LSDA profiles obtained from using the FN solution to the BA integral equations and from the present parameterization. The BALSDA/FVC and BALSDA/FN ground-state energies of the same system deviate from the DMRG energy by 0.01 and 0.64%, respectively. The local densities follow the same trend, and deviate from DMRG by 0.42 and 0.58%. For the local magnetization, the corresponding numbers are 2.20% for BALSDA/FVC and 5.86% for BALSDA/FN. Remarkably, for all three quantities the parameterized results are closer to the DMRG benchmark data than the numerically defined BALDA. This shows that the particular form chosen for the proposed parameterizations allows for considerable error cancellation. On 32 processors the DMRG calculation took approximately 17 h, whereas the BALSDA calculations required approximately 40 s. Of course, for high-precision calculations, as well as for the calculation of quantities that are not easily extracted from densities and energies, DMRG is still essential.

A more complex case is depicted in figure 5, which shows density and magnetization profiles for parabolically confined systems in a periodic chain. For two different values ($k = 0.05$ and $k = 0.5$) of the curvature of the confining potential (whose form is schematically indicated by the dashed (green) curve), the data points show the site-resolved particle density and spin density obtained by exact (Lanczos) diagonalization, FN BA-LSDA and our currently
Figure 4. (a) Density profile $n_i$ of an open chain with $L = 100$ sites, $N_\uparrow = 30$, $N_\downarrow = 20$ fermions, and $U = 4t$, obtained self-consistently from FN BALSDA, the present parameterization and DMRG calculations. (b) Local magnetization $m_i$ of the same system. Percentage deviations, summed over all sites, of the LSDA densities from the DMRG ones are given in parentheses.

Figure 5. Parabolically confined systems: (a) density profiles $n_i$ of periodic chains for two different values of curvature ($k = 0.05$ and $k = 0.5$). $L = 15$ sites, $N_\uparrow = 4$, $N_\downarrow = 3$ fermions, and $U = 4t$, obtained self-consistently from FN BALSDA, the present parameterization and exact (Lanczos) calculations. (b) Local magnetization $m_i$ of the same systems.

proposed parameterization. To within the accuracy that can be expected from an LDA for this type of system (a few per cent) the agreement between all three sets of calculations is excellent, for both charge and spin distributions. The amplitude of the magnetization-density oscillations is overestimated by both flavours of local approximations, which is consistent with previous observations for similar approximations and systems [20].
Figure 6. Per-site ground-state energy of finite open chains with $L = 15$ sites, $N_{\uparrow} = 4$ and $N_{\downarrow} = 3$ fermions, obtained self-consistently from FN BALSDA, the present parameterization and from exact diagonalization. Inset: BALSDA data for a larger chain with $L = 200$ sites, $N_{\uparrow} = 60$ and $N_{\downarrow} = 40$.

Next, we compare, in figure 6, the numerically exact ground-state energy obtained from Lanczos diagonalization of a small open Hubbard chain with $L = 15$ sites to the LSDA ground-state energies obtained using the FN solution to the BA integral equations and from using the present parameterization. Up to $U \sim 4t$ the BALSDA/FN data are almost identical to the exact data, which attests to the quality of the local approximation. For $U$ larger than $\sim 5t$, the present parameterization is once again better than the conceptually superior FN LSDA, due to error cancellation. The inset shows that for larger systems the behaviour is qualitatively the same.

Finally, we point out that the successful application of our (then unpublished) spin-dependent expression (11) to the study of spin-polarized transport across a correlated nanoconstriction [11] and to the calculation of occupation probabilities of exotic superfluids in spin-imbalanced systems [25] has already been reported.

5. Summary

In summary, we have constructed a simple and reliable parameterization for the ground-state energy of the homogeneous 1DHM, for arbitrary fillings, spin-polarizations and interactions. For the first time, a qualitatively and quantitatively correct description of the Mott gap is obtained from a simple density functional with a proper explicit derivative discontinuity. This parameterization can be used in its own right, for the homogeneous model, whenever simple expressions for the ground-state energy and for the resulting Mott gap are required.

However, its main application is as the input for LDA and LSDA, which allow one to efficiently minimize the energy and extract energies, density profiles and related quantities for spatially inhomogeneous models. Since in KS calculations one never diagonalizes the interacting Hamiltonian, but only the auxiliary noninteracting one, systems with thousands of sites can be dealt with, even in the absence of any simplifying symmetry.
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References

[1] Mott N 1990 *Metal–Insulator Transitions* 2nd sub-edn (Boca Raton, FL: CRC)
[2] Perdew J P, Parr R G, Levy M and Balduz J L Jr 1982 *Phys. Rev. Lett.* **49** 1691
[3] Mori-Sanchez P, Cohen A J and Yang W 2009 *Phys. Rev. Lett.* **102** 066403
[4] Mori-Sanchez P, Cohen A J and Yang W 2008 *Phys. Rev. Lett.* **100** 146401
[5] Cohen A J, Mori-Sanchez P and Yang W 2008 *Science* **321** 792
[6] Grünig M, Marini A and Rubio A 2006 *J. Chem. Phys.* **124** 154108
[7] Grünig M, Marini A and Rubio A 2006 *Phys. Rev. B* **74** 161103
[8] Lima N A, Silva M F, Oliveira L N and Capelle K 2003 *Phys. Rev. Lett.* **90** 146402
[9] Lima N A, Oliveira L N and Capelle K 2002 *Europhys. Lett.* **60** 601
[10] Kurth S, Stefanucci G, Khosravi E, Verdozzi C and Gross E K U 2010 *Phys. Rev. Lett.* **104** 236801
[11] Mirjani F and Thijssen J M 2011 *Phys. Rev. B* **83** 035415
[12] Akande A and Sanvito S 2010 *Phys. Rev. B* **82** 245114
[13] Schenk S, Dzierzawa M, Schwab P and Eckern U 2008 *Phys. Rev. B* **78** 165102
[14] Verdozzi C 2008 *Phys. Rev. Lett.* **101** 166401
[15] Capelle K, Lima N A, Silva M F and Oliveira L N 2003 *Prog. Theor. Chem. Phys.* **14** 145
[16] Silva M F, Lima N A, Malvezzi A L and Capelle K 2005 *Phys. Rev. B* **71** 125130
[17] Campo V L Jr and Capelle K 2005 *Phys. Rev. A* **72** R-061602
[18] França V V and Buchleitner A 2011 *Phys. Rev. B* **82** 075120
[19] Lieb E H and Wu T Y 1968 *Phys. Rev. Lett.* **20** 1445
[20] Essler F H et al 2005 *The One-Dimensional Hubbard Model* (Cambridge: Cambridge University Press)
[21] Schollmann P 1997 *Int. J. Mod. Phys. B* **11** 355
[22] França V V and Buchleitner A 2011 arXiv:1103.2951