Density-functional theory on a lattice: Comparison with exact numerical results for a model with strongly correlated electrons

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Most of the basic ideas of the density-functional theory (DFT) are shown to be unrelated to the fact that the particle density is used as the basic variable. After presenting the general formalism and a simple example unrelated to densities, we discuss various approaches to density-functional theory on a lattice. One has proven useful for the understanding of various fundamental issues of the DFT. The exact Kohn-Sham band gap and the band gap in the local-density approximation (LDA) are compared to the exact result for a one-dimensional model. As the interacting homogeneous system can be solved exactly no further approximation is needed to formulate the LDA.

I. INTRODUCTION

Density-functional theory[1,2] is the most successful method for *ab initio* calculations of electronic properties of solids. An important conceptional progress was the definition of the relevant functionals by Levy's constrained search method,[3] which will be used in the following. This approach can be used for a wide class of quantum mechanical problems, which involve an unperturbed Hamiltonian H_0 and a perturbation V. If one encounters the same *type* of perturbation very often, the same strategy as in the density-functional theory (DFT), where the same type of perturbation describes all molecules and solids in the Born-Oppenheimer approximation, can be used to approach the problem.

Despite the success of the DFT, some fundamental problems remain, like the question of the continuity of the exchange-correlation potential,[4,5] and the meaning of the Kohn-Sham (KS) eigenvalues.[6] In order to partly simplify these issues, two of us have introduced the equivalent of DFT on a lattice, where the local site occupancies were treated as the basic variables.[7–9] A different approach to the DFT on a lattice has been presented recently,[10] which insists on using the density $n(\mathbf{r})$, with $\mathbf{r}$ as a continuous variable even on a lattice. As the discussion in Sec. II will show, this misses a major point of our previous work.[7–9] Therefore, it is useful to present the following general approach, which provides a clear theoretical framework to compare the different approaches to DFT on a lattice. We show that only our previous approach is useful in discussing questions related to the KS eigenvalues. Exact numerical results are presented for a Hubbard chain in an alternating external field, using the density-matrix renormalization group (DMRG) approach.[11] For a small external field, this can be considered as a model of a Mott insulator and for a large field as a model of an ionic insulator. The exact gap for this model is compared to the exact KS band gap and the local-density approximation (LDA) band gap. It is a special feature of the model that no further approximation is necessary to set up the LDA, as the homogeneous system can be solved exactly using the Bethe-Ansatz.[12,13]

II. $\{A\}$-FUNCTIONAL THEORY

We consider a Hamiltonian of the type

$$H = H_0 + \sum_i \lambda_i \hat{A}_i, \tag{1}$$

where the label i in the operator $\hat{A}_i$ can be discrete or continuous. Usual DFT corresponds to the continuous case with $\hat{A}_i \to \hat{n}(\mathbf{x})$ and $\lambda_i \to V(\mathbf{x})$, where $V(\mathbf{x})$ is the external potential. Other choices of variables are, e.g., spin densities,[2,14] current densities,[15] anomolous densities for superconducting sytems[16] and pair densities.[17]

The expectation values of $\hat{A}_i$ in a normalized state $|\phi\rangle$ are denoted by $a_i(\phi)$

$$a_i(\phi) \equiv \langle\phi|\hat{A}_i|\phi\rangle, \quad i = 1, 2 \ldots . \tag{2}$$

In the spirit of Levy,[3] we define $M(\{a\})$ as the set $\{|\phi\{a\}\rangle\}$ of all states, which lead to the same set $\{a\}$ of expectation values. The expectation value of H_0 in these states is, in general, different. The smallest possible value of $\langle\phi\{a\}|H_0|\phi\{a\}\rangle$ is denoted by $F(\{a\})$,

$$F(\{a\}) \equiv \min_{|\phi\rangle \in M(a)} \langle\phi\{a\}|H_0|\phi\{a\}\rangle \ . \tag{3}$$

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This is a function in the discrete case and a functional in the continuous case. In the following, we always use the term functional. Next we define the functional $E(\{a\})$,

$$E(\{a\}) \equiv F(\{a\}) + \sum_i \lambda_i a_i \ . \tag{4}$$

Now Levy's version of the basic strategy can be used.

Let $|\phi_{\min}\{a\}\rangle \in M(a)$ be the (or one of the) state(s) that yield(s) the smallest expectation value for H_0. Then we have

$$\begin{aligned}\langle\phi_{\min}\{a\}|(H_0 + \sum_i \lambda_i \hat{A}_i)|\phi_{\min}\{a\}\rangle \\ = F\{a\} + \sum_i \lambda_i a_i = E(\{a\}) \ .\end{aligned} \tag{5}$$

Since for every state $|\psi\rangle$, one has $\langle\psi|H|\psi\rangle \geq E_0$, where E_0 is the ground-state energy, the inequality

$$E(\{a\}) \geq E_0 \tag{6}$$

follows.

If the (or one of the) ground state(s) of H is denoted by $|\psi_0\{\lambda\}\rangle$ and its expectation values of the $\hat{A}_i$ are denoted by a_i^0, the definition Eq. (3) leads to $\langle\psi_0\{\lambda\}|H|\psi_0\{\lambda\}\rangle \geq F(\{a_i^0\})$, i.e.,

$$\begin{aligned}E_0 &= \langle\psi_0\{\lambda\}|H_0|\psi_0\{\lambda\}\rangle + \sum_i \lambda_i a_i^0 \\ &\geq F(\{a_i^0\}) + \sum_i \lambda_i a_i^0 = E(\{a^0\}),\end{aligned} \tag{7}$$

which is the second inequality of the "$\{a\}$-functional theory"

$$E_0 \geq E(\{a^0\}). \tag{8}$$

In order to avoid the contradiction between (6) and (8), we can combine them in the relation

$$E(\{a\}) \geq E(\{a^0\}) = E_0. \tag{9}$$

Like in the usual DFT theory, this is the central result of $\{a\}$-functional theory. If the functional $F(\{a\})$ can be computed, the ground-state energy and the ground-state expectation values $\{a^0\}$ can be obtained by minimizing $E(\{a\})$. This leads to the Euler equation

$$\delta F(\{a\})/\delta a_i + \lambda_i = 0 \ . \tag{10}$$

Obviously, the difficult task of solving always the Schrödinger equation $H|\psi_0\rangle = E_0|\psi_0\rangle$ for a given set of $\{\lambda\}$ is avoided, but only at the expense of determining the functional $F(\{a\})$. This is, in general, as complicated as the complete solution of the Schrödinger equation. Only in very simple cases, such as the one discussed at the end of this section, can the exact functional $F(\{a\})$ be found by actually performing the constrained search without solving a Schrödinger equation. Generally, it is impossible to obtain the exact expression for the functional $F(\{a\})$. The use of the $\{a\}$-functional theory is, therefore, only profitable if clever approximations for $F(\{a\})$ can be found, as in the usual DFT. The general formulation as presented above shows that the approach provides *no* hint about how to obtain ground-state expectation values of operators *different* from $\hat{A}_i$ and the Hamiltonian H.

Another important aspect of DFT is the seminal idea of Kohn and Sham[2] to make a shift to a system of noninteracting electrons, which is based on the assumption that the ground-state density of the interacting system can also be generated by noninteracting electrons in an appropriate potential. In our general framework, this can be described as follows. Let $\tilde{H}_0$ be different from H_0 and $|\tilde{\psi}_0\{\tilde{\lambda}\}\rangle$ the ground state of $\tilde{H} = \tilde{H}_0 + \sum_i \tilde{\lambda}_i \hat{A}_i$. We *assume* that $\tilde{H}_0$ is such that $\tilde{\lambda}_i$ can be found, which fulfill

$$\langle\psi_0\{\lambda\}|\hat{A}_i|\psi_0\{\lambda\}\rangle = \langle\tilde{\psi}_0\{\tilde{\lambda}\}|\hat{A}_i|\tilde{\psi}_0\{\tilde{\lambda}\}\rangle \tag{11}$$

for all i. If we write the Euler equation (10) in the form

$$\frac{\delta\tilde{F}}{\delta a_i} + \left(\frac{\delta F}{\delta a_i} - \frac{\delta\tilde{F}}{\delta a_i} + \lambda_i\right) = 0, \tag{12}$$

where $\tilde{F}$ is the $\{a\}$-functional corresponding to $\tilde{H}$, we can view (12) as the Euler equation for the $\{a\}$-functional theory corresponding to $\tilde{H}$ if we identify $\tilde{\lambda}_i$ with the expression in the parentheses. Instead of solving Eq. (10) in order to obtain the ground-state expectation values a_i^0, we can alternatively solve the Schrödinger equation,

$$\left[\tilde{H}_0 + \sum_i \left(\frac{\delta(F-\tilde{F})}{\delta a_i} + \lambda_i\right)\hat{A}_i\right]|\tilde{\psi}_0\rangle = \tilde{E}_0|\tilde{\psi}_0\rangle, \tag{13}$$

together with the self-consistency relation,

$$\left\langle\tilde{\psi}_0\left\{\lambda + \frac{\delta(F-\tilde{F})}{\delta a}\right\}\middle|\hat{A}_i\middle|\tilde{\psi}_0\left\{\lambda + \frac{\delta(F-\tilde{F})}{\delta a}\right\}\right\rangle = a_i. \tag{14}$$

This approach is favorable if $\tilde{H}_0$ is *simpler* than H_0, and if approximations for the *difference* $F - \tilde{F}$ can be found that are better than the approximations for the separate pieces. It was another important insight of Kohn and Sham[2] to realize that this is the case in the usual DFT when the kinetic energy is chosen as $\tilde{H}_0$. The problem to be solved is then one of *noninteracting* electrons in an effective potential. For a crystalline solid, this brings in all the concepts of band theory. But one has to keep in mind that the one-electron eigenvalues have no obvious direct meaning. In order to clarify the nature of the one-electron eigenvalues with the help of DFT on a lattice, it is important to make sure that Eq. (11) is fulfilled when one decides which term in the Hamiltonian is considered the external perturbation.

Before we discuss the DFT on a lattice in Sec. III, we present a very simple example of the approach described, the "$\langle x^2\rangle$-functional theory" of the harmonic oscillator.

We consider the harmonic oscillator

$$H = \frac{\hat{p}^2}{2m} + \frac{1}{2}m\omega_0^2\hat{x}^2 \equiv H_0 + \lambda\hat{x}^2. \tag{15}$$

In this simple example, the function $F(x^2)$ can be calculated exactly, as the Heisenberg uncertainty relation ($x^2 \equiv \langle\hat{x}^2\rangle$) can be used in the constrained search. One obtains

$$F(x^2) = \frac{1}{2m} \min_{|\phi\rangle \in M(x^2)} \langle\phi(x^2)|\hat{p}^2|\phi(x^2)\rangle = \frac{1}{2m}\frac{(\hbar/2)^2}{x^2}. \tag{16}$$

The x^2-energy functional is then given by

$$E(x^2) = \frac{1}{2m}\frac{(\hbar/2)^2}{x^2} + \frac{1}{2}m\omega_0^2x^2 , \tag{17}$$

and the minimization $\delta E/\delta x^2 = 0$ immediately leads to the well-known answers $(x^2)^0 = \hbar/(2m\omega_0)$ and $E_0 = \hbar\omega_0/2$.

In contrast to the usual DFT, the energy functional can be calculated exactly in this example. Closer in spirit to the problem one encounters with approximations for $F(\{a\})$ is the x^2-functional theory of a quartic anharmonic oscillator with

$$H_0 = \frac{1}{2m}\hat{p}^2 + e^2\hat{x}^4, \tag{18}$$

where e^2 is the fixed coupling constant of the quartic term. Now $F(x^2)$ can, for example, be calculated approximately by using a search in a restricted class of functions.

III. DFT ON A LATTICE

In order to gain insight into the "band-gap" problem,[7,8] and for comparing the Kohn-Sham Fermi surface with the exact quasiparticle Fermi surface,[9] we previously introduced the concept of a DFT on a lattice. As is obvious from Sec. II, there is an enormous freedom how to split up the Hamiltonian on the lattice in the form (1) and, therefore, there are many different $\{a\}$-functional theories for treating the problem.

We used Hubbard type single (or two) band models in external potentials $V_{i\sigma}$, e.g.,

$$H = \sum_{\langle i,j\rangle\sigma} t_{ij}c_{i\sigma}^\dagger c_{j\sigma} + U\sum_i n_{i\uparrow}n_{i\downarrow} + \sum_{i\sigma} V_{i\sigma}n_{i\sigma}, \tag{19}$$

where for simplicity we used the on-site Coulomb repulsion U and the hopping matrix elements t_{ij} independent of the potential V_i. Then a natural choice for a generalized DFT is $\hat{A}_i \to n_{i\sigma}$ (or $\hat{A}_i \to n_{i\uparrow} + n_{i\downarrow}$ if $V_{i\sigma} = V_i$, independent of σ), i.e., the local site occupancies are treated as the basic variables. In this way, the three-dimensional continuous variable $\rho(\mathbf{x})$ in the usual DFT is replaced by the three-dimensional discrete variable $n_{i\sigma}$. This is the approach we used earlier.[7–9] To distinguish it from the usual DFT, we call this approach *site occupation function(al) theory* (SOFT) in the following. In order to address questions concerning the one-electron KS eigenvalues, we chose the kinetic energy [first term on the rhs of Eq. (19)] as $\tilde{H}_0$ and presented strong *numerical evidence* that the site occupancies $\langle n_{i\sigma}\rangle$ are *noninteracting v representable*, i.e., Eq. (11) is fulfilled.

According to the discussion presented in Sec. II, it is obvious that *other* choices of the perturbation are perfectly possible. If one takes only the second term on the right-hand side of Eq. (19), the Coulomb term, as the unperturbed Hamiltonian H_0, all $\langle c_{i\sigma}^\dagger c_{j\sigma}\rangle$ are the basic variables of the corresponding {a}- functional theory. It was shown recently by Schindlmayr and Godby[10] using a numerical study of finite one-dimensional clusters that the resulting theory is *not* noninteracting v repesentable. It is impossible for noninteracting electrons to reproduce *all* expectation values $\langle c_{i\sigma}^\dagger c_{j\sigma}\rangle$ of the interacting system, which exhibit correlation-induced localization. While this is interesting in itself, it also shows that this decomposition should *not* be used if one wants to obtain deeper understanding of problems related to the KS eigenvalues.

We, therefore, stick to the SOFT used in our earlier publications[7–9] and present results for a one-dimensional model. We consider an a-b Hubbard chain (19) with the external potential $V_i = (-1)^i(\delta/2)$ at half-filling. We keep only nearest neighbor matrix elements $t_{i,i\pm1} \equiv t$. The homogeneous system ($\delta = 0$) can be solved *exactly* for finite U, using the Bethe-Ansatz method.[12,13] This allows us to set up an exact LDA discussed later. For $\delta \neq 0$, only the noninteracting case $U = 0$ and the atomic limit $t = 0$ can be solved analytically. For $U = 0$, the system is a semiconductor with energy bands $\epsilon_{k,\pm} = \pm\sqrt{4t^2\cos^2k + (\delta/2)^2}$, i.e., the gap is given by $|\delta|$. The difference of the occupancies on the a and b sites follows from filling the lower band,

$$\frac{n_a - n_b}{2} = \int_{-\pi/2}^{\pi/2} \frac{\delta/2}{\sqrt{4t^2\cos^2k + (\delta/2)^2}}\frac{dk}{\pi} \equiv f(\delta). \tag{20}$$

Here, the function f is a monotonously increasing odd function with $f \to 1$ as the argument goes to infinity.

For finite values of the on-site Coulomb repulsion U, we have used the density-matrix formulation of the numerical renormalization group.[11] This allows us to treat one-dimensional systems of sizes much larger than is possible using exact diagonalization. As the method works best with open boundary conditions, we have used these for chains up to $N_s = 64$ sites. As a function of the chain length, the difference of the occupancy of the a and b sites in the middle of the chain converges rapidly to the infinite chain limit. For $\delta = U = 4$, for example, we find that for $N_s = 16$, 32, and 64, $n_a = 1.4986$, $n_a = 1.500\,35$, and $n_a = 1.500\,39$, respectively. The exact band gap defined in terms of the exact ground-state energy $E_0(N)$ for N electrons,

$$E_g = E_0(N_s + 1) + E_0(N_s - 1) - 2E_0(N_s), \tag{21}$$

shows a similar rapid convergence with increasing chain length.

For a given value of δ, the exact band gap E_g is nonmonotonic as a function of U. The behavior for small U can be understood easily in terms of the (restricted) Hartree-Fock (HF) approximation valid in this regime. The effective site energy on the a sites ($V_a = -\delta/2 < 0$) is given by $-\delta/2 + Un_a^{\rm HF}/2$. The HF gap for the one-dimensional chain is then $E_g^{\rm HF} = \delta - U(n_a^{\rm HF} - n_b^{\rm HF})/2$, i.e., the exact gap and the HF gap both *decrease linearly* with U for small U, as shown in Fig. 1. Here, we use $|t| = 1$ as the energy unit. For $U \gg |t|$, a simple expression for E_g can again be obtained. For $N = N_s$ and $U \gg \delta$, the ground-state energy can be approximated by the result for the Heisenberg antiferromagnet,[13] $E_0(N_s) \approx -N_s 4\ln 2(t^2/U)$. The $N_s \pm 1$ ground-state problem is closely related to the Nagaoka problem[18] of a single electron (hole) in a ferromagnetic background. This leads to

$$E_g \approx U - 2\sqrt{4t^2 + (\delta/2)^2} + 8\ln 2(t^2/U) \ , \qquad (22)$$

i.e., a *linear increase* of the gap for $U \gg (|t|, |\delta|)$. For $U = 20$, this approximate expression yields a gap of 14.62, very close to the result 14.57 from the DMRG calculation. A third analytical tool to understand the qualitative behavior of $E_g(U, t, \delta)$ is the atomic limit $t \to 0$. For $U < \delta$ and $N = N_s$ the ground state consists of doubly occupied sites and $E_g(U, 0, \delta) = \delta - U$. For $U > \delta$ and $N = N_s$, all sites are singly occupied and one obtains $E_g(U, 0, \delta) = U - \delta$. For $U \ll \delta$ and $U \gg \delta$, these results agree with the approximations discussed earlier. For finite t one, therefore, expects a minimum of the gap for U somewhat larger than δ. This is what the exact results in Fig. 1 (squares) show.

The difference of the occupancies on the a and b sites decreases monotonously with increasing U, with the most rapid decrease for $U \approx \delta$, when the energy of a doubly occupied a site and an empty b site is degenerate with singly occupied a and b sites. The exact results are shown as squares in Fig. 2.

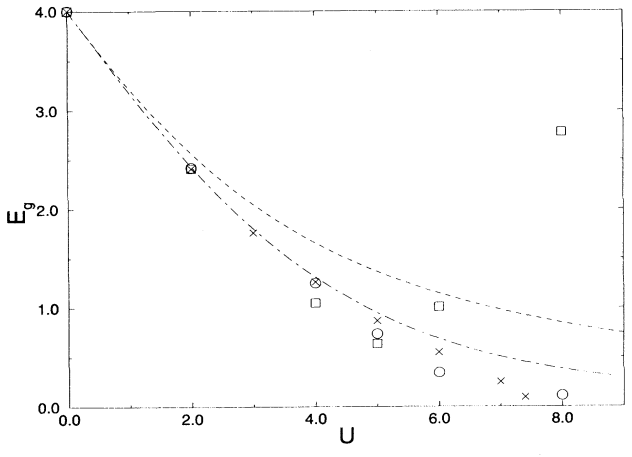

FIG. 1. Energy gap as defined in Eq. (21) as a function of U for fixed $\delta = B = 4$. The exact DMRG results are presented by squares, the exact KS gap by circles, and the LDAE gap by crosses. The dotted line shows the HF- and the dashed-dotted line the LDA2 results.

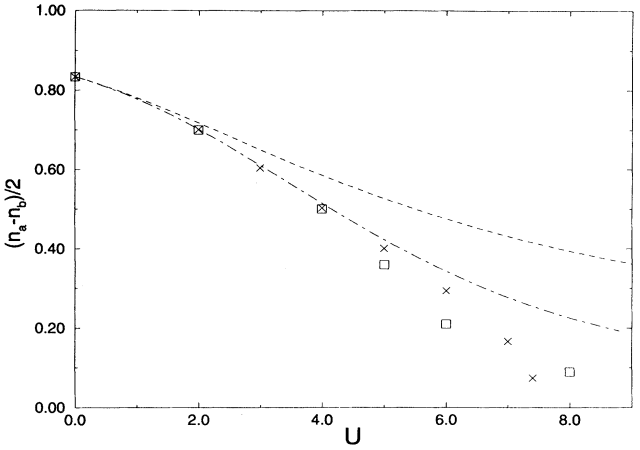

FIG. 2. Difference of site occupancies for the parameters of Fig. 1. As the exact KS results agree by definition with the exact results, no circles are shown. Otherwise, the various results are presented by the same symbols as in Fig. 1.

Once we have exact results for the occupancies we can, using Eq. (20), determine the exact KS potential $V_{i,\rm eff} = (-1)^i(\delta_{\rm eff}/2)$, which leads to the *same* occupancies for a system of noninteracting electrons. The corresponding KS gap, which follows from the (incorrect) *assumption* that $V_{i,\rm eff}$ is *continous* as a function of particle number, is then given by $|\delta_{\rm eff}|$. The results are shown as circles in Fig. 1. For $U \ll \delta$ the KS gap and the exact gap are in excellent agreement, while for $U \gg \delta$ there is a large discrepancy. This is due to the discontinuity of the exchange-correlation potential.[4] For $\delta = 0$, this example of the discontinuity has been discussed earlier.[7]

Many features of these results can already be seen for the *two site* chain. Apart from the fact that the KS gap for $N_s = 2$ is always smaller than the exact gap, the $N_s = 2$ results, which require only the diagonalization of a 3×3 matrix, show the same qualitative behavior as the results discussed above and shown in Figs. 1 and 2.

IV. LOCAL APPROXIMATIONS

In order to illustrate with our model the approach usually taken in DFT, we have to provide approximations within SOFT for the function(al) F, or the difference $F - \tilde{F}$, when we work with the KS scheme described in Eqs. (13) and (14). The difference $F - \tilde{F}$ is the sum of the Hartree- and the exchange-correlation (xc) functional, as we choose $\tilde{H}_0$ to be the kinetic energy term in Eq. (19). The standard approximation for the xc functional is the LDA (Ref. 6) (possibly with gradient corrections). In DFT, no exact solution for the homogeneous electron gas is available, but it should be pointed out that in modern parametrizations[19,20] of the Monte Carlo results[21] for jellium, the errors are negligible for most systems compared to the errors inherent in the LDA. Nevertheless, it is a

nice feature of the model dicussed above that we are able to obtain the *exact* LDA. The homogeneous case corresponds to the one-dimensional Hubbard model, which can be solved exactly by the Bethe-Ansatz method.[12] We shortly summarize the results needed later.

To obtain the exact ground-state energy for arbitrary band filling $n \equiv N/N_s$, the Lieb-Wu integral equation[12] for the distribution function $\rho(k)$ has to be solved numerically. This was first done by Shiba.[13] For the discussion of the results, it is useful to add an energy $-U/2$ at each site, which makes the results particle-hole symmetric; i.e., the ground-state energy per site $\epsilon_0 \equiv E_0(N)/N_s$ is an *even* function of $(n-1)$. The results for $U = 4|t| \equiv B$ are shown in Fig. 3. For comparison, we also show the result for the HF approximation and from a ground-state energy calculation up to second order in U.[22] The latter provides an important improvement over the HF result, but this improvement is *not uniform in n*.

The quantity that enters the LDA discussed below is the derivative $\epsilon_0'(n) \equiv d\epsilon_0(n)/dn$, which is an *odd* function of $(n-1)$. As first realized by Lieb and Wu,[12] the function ϵ_0' has a *discontinuity* at $n = 1$ for *all* values of $U > 0$. For $U \ll |t|$, the corresponding gap is *exponentially small*, while it increases linearly with U for large U. For space dimensions larger than one, the large U behavior is similar, but the gap is generally believed to be zero for $U < U_c \sim B$, where B is the bandwidth. As we have not found a plot of the gap as a function of U in the literature, we show it in Fig. 4. Also shown is the expression presented in Eq. (22), which provides an excellent approximation for $U > B$.

In order to obtain numerical data for $\epsilon_0'(n)$, we have solved the Lieb-Wu integral equation[12] in the same manner as Shiba,[13] using a discretization method and have obtained $\epsilon_0'(n)$ by numerical differentiation. The result for $\epsilon_{\rm int}'(n) \equiv \epsilon_0'(n,U) - \epsilon_0'(n,0)$ for $U = B$ is shown in Fig. 5. For comparison, we again show the result for the HF approximation $[(\epsilon_{\rm int}'(n)^{\rm HF} = U(n-1)/2]$ and from the ground-state energy calculation up to second order in U.[22] Due to the nonuniformity of the improvement in n, the latter yields a reasonable approximation only for intermediate values of the filling, but shows qualitatively wrong behavior for $n \ll 1$ and $n \approx 1$. It does not produce the gap at $n = 1$. In fact, the gap does not show up in any order perturbation theory, which provides only an *asymptotic* series for small U.[22] The exact results for $\epsilon_{\rm int}'(n)$ for various values of U are shown in Fig. 6.

Within SOFT the *exact* LDA is obtained by $V_{i,\rm eff} = V_i + \epsilon_{\rm int}'(n_i)$, together with the self-consistency relation (14) for the site occupancies n_i. In the usual nomenclature, $\epsilon_{\rm int}'(n)$ is the *sum* of the Hartree and the xc

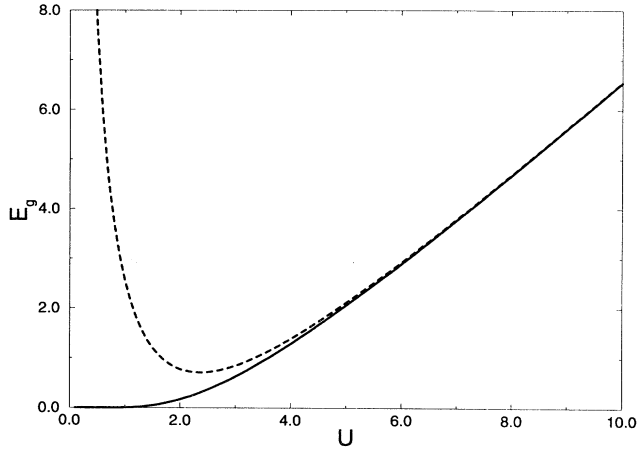

FIG. 4. Energy gap for $\delta = 0$ and $|t| = 1$ as a function of U. The full line presents the exact Lieb-Wu result and the dashed curve shows the approximation given by Eq. (22).

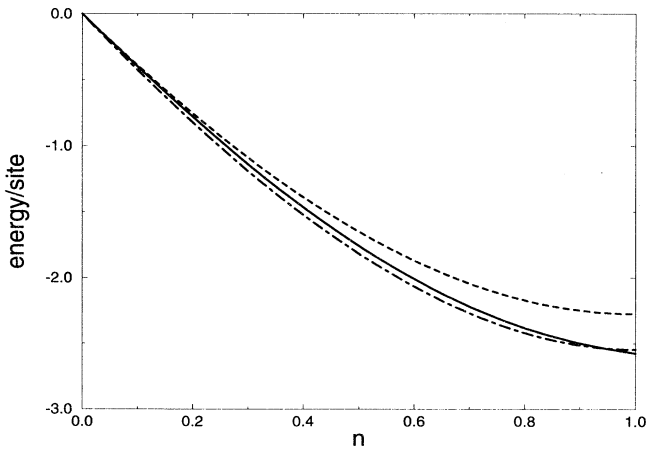

FIG. 3. Ground-state energy per site for $\delta = 0$, as a function of $n = N/N_s$. The full curve presents the exact solution from the Lieb-Wu integral equation, the dashed curve shows the HF result, and the dashed-dotted curve perturbation theory to second order in U. Note that the site energies have been chosen such that the result is particle-hole symmetric.

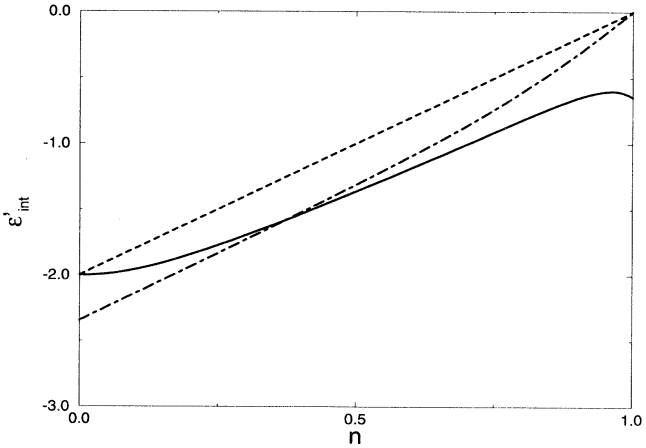

FIG. 5. Sum of the Hartree and the xc potential as a function of n. The curves result from differentiation of the corresponding curves in Fig. 3, with respect to n.

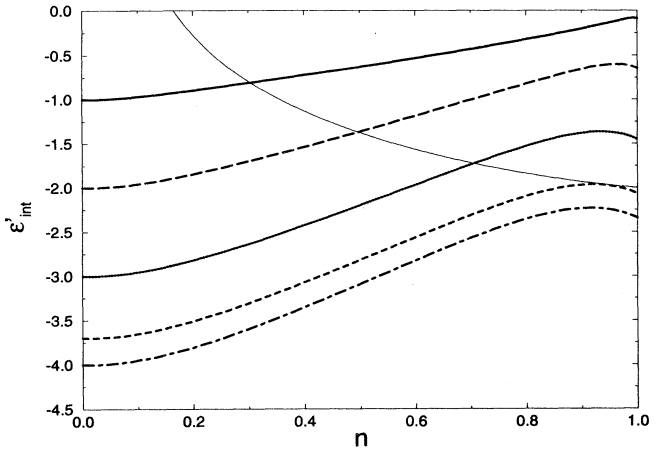

FIG. 6. Exact results for the sum of the Hartree and xc potential as a function of n for various values of U : $U = 2$ (full line); $U = 4$ (long dashed line); $U = 6$ (dotted line); $U = 7.4$ (dashed line); and $U = 8$ (dashed-dotted line). The thin full line presents $[-\delta + f^{-1}(1-n)]/2$ and the crossings correspond to the self-consistent solutions.

potential. For the a-b chain the self-consistency condition reduces to Eq. (20) with δ replaced by $\delta_{\rm eff} = \delta - \epsilon'_{\rm int}(n_a) + \epsilon'_{\rm int}(n_b)$. In the half-filled band case this reads

$$\delta + 2\epsilon'_{\rm int}(1-q) = f^{-1}(q), \tag{23}$$

where $q \equiv (n_a - n_b)/2$ and f^{-1} is the inverse of the function defined in Eq. (20). The qualitative behavior of the results follows easily from a graphical solution of this equation.

We have performed three types of LDA calculations corresponding to the three curves shown in Fig. 5. In SOFT the HF approximation for the model (19) corresponds to the *exchange only* LDA. The HF results are shown as the dashed lines in Figs. 1 and 2. The HF gap is always larger than the KS gap. For $U \ll \delta$ it approaches the exact result, but for $U \to \infty$, it goes to zero as the KS gap. This unphysical behavior occurs because the (restricted) HF approximation is unable to incorporate the strong antiferromagnetic correlations, which exist in this limit. Within an unrestricted HF calculation which allows $\langle n_{i,\uparrow}\rangle^{\rm HF} \neq \langle n_{i,\downarrow}\rangle^{\rm HF}$, an approximate description of these correlations is possible. There is no such symmetry breaking in the exact solution.

For not too large values of U and densities not close to $n = 0$ or $n = 1$, the result for $\epsilon'_{\rm int}(n)$ from second order perturbation theory in U provides a definite improvement over the HF result. The self-consistent LDA with this approximation for $\epsilon'_{\rm int}$ (LDA2) therefore leads to significant improvements for the values of the gap and the occupancies for $U < \delta$. This is shown in Figs. 1 and 2, where the LDA2 results correspond to the dashed-dotted line.

The *exact* LDA results (LDAE) are obtained using the *exact* results for $\epsilon'_{\rm int}$. A surprising feature of these calculations, which probably has the same origin as the instability of the restricted HF solutions for large U, is the fact that *no self-consistent solutions exist for values of U larger than a critical value* $U(\delta)$. This can easily be seen from Fig. 6, where the thin full line presents $[-B + f^{-1}(1-n)]/2$ and the crossings with the $\epsilon'_{\rm int}(n)$ curves yield the self-consistent solutions for $\delta = B$. For $\delta = B = 4$, the critical value of U above which no solutions exist is approximately given by 7.4 . As $\epsilon'_{\rm int}(n)$ is nonmonotonic in n, there is a small region below $U(\delta)$, where *two* self-consistent solutions exist. In Figs. 1 and 2, the LDAE results are presented as crosses. In the range where LDAE solutions exist, the results show a further improvement over the LDA2 results and for $U < \delta$ the agreement with the exact results for $(n_a - n_b)/2$ is excellent. For values $U > 6$ the discrepancy of the exact gap to the SOFT results becomes large. This is due to the discontinuity of the xc functional. For $U = 6$ the HF gap is larger than the exact gap, while the the LDAE gap is smaller as it is typical for real insulators. The LDAE gap is closer to the KS gap than to the exact result.

V. SUMMARY

We have presented a formulation of the general framework that lies behind DFT. This was used as a setting to discuss various approaches to density-functional theory on a lattice. The choice of using the site occupancies as the basic variables (SOFT) has turned out to be useful in addressing fundamental questions of DFT in the KS scheme, such as the meaning of the one-electron eigenvalues, given the prerequisite of noninteracting v representability. One of the successes of this approach was the first demonstration that the exact KS-Fermi surface differs from the exact quasiparticle Fermi surface, which also stimulated a counterexample in the usual DFT.[23] Here we have treated a one-dimensional model, which may simulate a Mott insulator or an ionic insulator, depending on the value of the alternating potential. The LDA was formulated without further approximations. Comparison of the exact gap with the exact KS gap and the LDAE gap showed that there are parameter ranges where the difference of the LDAE gap from the exact gap is mainly due to the discontinuity of the xc functional.

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