PHYSICAL REVIEW B **79**, 235101 (2009)

Scaling and transferability of the interaction-energy functional of the inhomogeneous Hubbard model

Matthieu Saubanère and G. M. Pastor
Institut für Theoretische Physik, Universität Kassel, Heinrich Plett Straße 40, 34132 Kassel, Germany
(Received 6 February 2009; published 1 June 2009)

The inhomogeneous Hubbard model is investigated in the framework of lattice density-functional theory (LDFT) by considering the single-particle density matrix γ_{ij} with respect to the lattice sites as the basic variable of the many-body problem. The domain of representability of γ_{ij} is determined for charge-density wave states on finite bipartite lattices. Levy's constrained search of the interaction-energy functional $W[\gamma_{ij}]$ is numerically solved by applying the Lanczos method to an effective Hubbard-type model. The exact functional dependence of $W[\gamma_{ij}]$ is analyzed by varying systematically the charge transfer $\Delta n=\gamma_{22}-\gamma_{11}$, the degree of electron delocalization g_{12} between the sublattices, the number of sites N_a, and the band filling $n=(\gamma_{11}+\gamma_{22})/2=N_e/N_a$. For each Δn the properties of W are discussed in the limits of weak ($\gamma_{12}\simeq\gamma_{12}^{0}$) and strong ($\gamma_{12}\simeq\gamma_{12}^{\infty}$) electronic correlations, as well as in the crossover region ($\gamma_{12}^{\infty}\leq\gamma_{12}\leq\gamma_{12}^{0}$). It is shown that W follows quite closely a simple scaling behavior as a function of Δn and $g_{12}=(\gamma_{12}-\gamma_{12}^{\infty})/(\gamma_{12}^{0}-\gamma_{12}^{\infty})$. The very good transferability of $W(\Delta n,g_{12})$ for different N_a, n and lattice structure opens new possibilities of applying LDFT to inhomogeneous many-body models.

DOI: 10.1103/PhysRevB.79.235101 PACS number(s): 71.15.Mb, 71.10.Fd, 71.45.Lr, 71.27.+a

I. INTRODUCTION

The density-functional approach to the inhomogeneous electron gas has been the subject of remarkable advancements since its original formulation by Hohenberg and Kohn.[1] After formal developments, extensions, and uncountable successful applications to a wide variety of problems, the theory has steadily grown into the most efficient method of determining electronic properties of matter from first principles.[2,3] In practice the calculations are, generally, based on the Kohn-Sham (KS) scheme which implements the variational principle in terms of the electronic density $\rho(r)$ by reducing the correlated many-body problem to the solution of a set of self-consistent single-particle equations.[4] While this transformation is formally exact, the actual computations always involve approximations to the interaction-energy functional $W[\rho]$ that condition the quality of the final results. The most extensively used forms for $W[\rho]$ are the local density approximation (LDA),[4] its spin-polarized version or local spin-density approximation (LSDA),[5] and the gradient-corrected extensions or generalized gradient approximations (GGAs),[6] which were originally derived from exact results for the homogeneous electron gas. Despite their extraordinary success in the most diverse areas, the LDA- and GGA-based approaches fail systematically in accounting for strong electron-correlation effects as observed, for example, in Mott insulators, heavy-fermion materials, or high-T_c superconductors.[7,8] Explaining these phenomena from first principles constitutes one of the major current challenges in condensed-matter theory.

Strongly correlated systems are usually described in the framework of lattice Hamiltonians such as Anderson,[9] Hubbard,[10] Pariser-Parr-Pople,[11] and related models, which focus on the most relevant electron dynamics at low energies. A detailed understanding of strong electron-correlation effects remains a very difficult task even if advantage is taken from the model simplifications. Exact results are rare or numerically very demanding. Therefore, a variety of elaborate many-body techniques has been specifically developed in order to study this problem. Being in principle an exact universally applicable theory, the limitations of density-functional theory (DFT) must be ascribed to the approximations used for the exchange and correlation energies and not to the underlying formalism. It is, therefore, important to extend the scope of DFT to investigations of many-body lattice Hamiltonians. Besides the theoretical interest of the model physics, such developments are very attractive since they provide a real alternative to the LSDA and related gradient-corrected methods. They open new insights into the properties of W, which should also be relevant for applications to increasingly realistic Hamiltonians or even first-principles calculations.

In past years a number of investigations have been performed by applying the concepts of DFT to lattice models. The studied problems include the determination of band gaps in semiconductors,[12] the role of off-diagonal elements of the density matrix and the noninteracting v representability in strongly correlated systems,[13] the development of energy functionals of the density matrix with applications to Hubbard and Anderson models,[14] studies based on the exact solution of the one-dimensional (1D) Hubbard model,[15] and most recently investigations of time-dependent effects.[16] The background of the present investigations is given by previous developments of lattice density-functional theory (LDFT) of many-body models and its applications to the Hubbard Hamiltonian in different dimensions.[17–20] In this approach the basic variable of the many-body problem is the density matrix γ_{ij}, where i and j refer to the lattice sites and the interaction energy W is regarded as a functional of γ_{ij}. Exact numerical results have been obtained for $W[\gamma_{ij}]$ of the Hubbard model on various periodic lattices having $\gamma_{ij}=\gamma_{12}$ for first nearest neighbors (NNs).[17] On this basis, a simple general approximation to $W(\gamma_{12})$ has been derived which incorporates the scaling properties of W, its analytical dimer ex-

pression, and known limits. Several electronic properties of 1D, two-dimensional (2D), and three-dimensional (3D) Hubbard models have been subsequently obtained in good agreement with available analytical Lanczos or Monte Carlo results. These include in particular the ground-state kinetic and correlation energies, charge-excitation gaps,[18] dimerization energies,[19] and charge susceptibilities.[20] LDFT appears, therefore, as an efficient method of determining the electronic properties of many-body lattice models.

A common feature of previous LDFT investigations is the restriction to systems showing a uniform distribution of the ground-state electron density. This allows one to assume that γ_{ii} is independent of i and to ignore their contribution to the functional dependence of W, except for the dependence on band filling. Although lattice models are based on localized orbitals and thus provide a real alternative to the electron gas approach, it is also true that the actual breakthrough of the Hohenberg-Kohn-Sham theory is its unique ability to cope with inhomogeneous $\rho(r)$.[1–4] One would, therefore, like to extend LDFT in order to understand the properties of $W[\gamma_{ij}]$ in the presence of inhomogeneous charge distributions. It is the purpose of this paper to investigate the Hubbard Hamiltonian on binary 1D lattices and to determine the exact dependence of W on the degree of charge transfer and electron delocalization, as obtained from Levy's constrained-search formulation and Lanczos diagonalization method.[21,22]

The remainder of the paper is organized as follows. In Sec. II the general background on LDFT is briefly recalled by pointing out the extensions involved in inhomogeneous models. Section III describes the numerical procedure used for calculating the interaction-energy functional $W[\gamma_{ij}]$. In Sec. IV the domain of representability of γ_{ij} is determined in the presence of charge-density waves (CDWs). Density matrices derived from the ground state of the Hubbard model (i.e., pure-state v representable γ_{ij}) as well as from more general N-particle states (i.e., N representable γ_{ij}) are considered. In Sec. V the exact functional dependence of $W[\gamma_{ij}]$ is determined as a function of the charge transfer between the sublattices and of the degree of electron delocalization. The scaling behavior and transferability properties are demonstrated by varying systematically the number of lattice sites N_a and band filling $n=N_e/N_a$. Finally, Sec. VI summarizes the main conclusions and points out some relevant future extensions.

II. DENSITY-FUNCTIONAL THEORY OF THE INHOMOGENEOUS HUBBARD MODEL

In order to be explicit we focus on the inhomogeneous Hubbard model which is expected to capture the main interplay between electronic correlations and charge-density redistributions. The Hamiltonian is given by

$$\hat{H} = \sum_{i,\sigma} \varepsilon_i \hat{n}_{i\sigma} + \sum_{\langle i,j\rangle\sigma} t_{ij} \hat{c}^{\dagger}_{i\sigma} \hat{c}_{j\sigma} + U \sum_{i} \hat{n}_{i\downarrow} \hat{n}_{i\uparrow}, \tag{1}$$

where ε_i denotes the site-dependent energy levels, t_{ij} is the NN hopping integrals, and U is the on-site interaction.[10] As usual $\hat{c}^{\dagger}_{i\sigma}$ ($\hat{c}_{i\sigma}$) stands for the creation (annihilation) operator for an electron with spin σ at site i ($\hat{n}_{i\sigma}=\hat{c}^{\dagger}_{i\sigma}\hat{c}_{i\sigma}$). The values of ε_i and t_{ij} define the distribution of different elements in the lattice, its dimensionality and structure, and the range of the single-particle hybridizations (typically, $t_{ij}=-t<0$ for NN ij). They specify the system under study and thus play the role given in conventional DFT to the external potential $v_{\text{ext}}(\vec{r})$. Consequently, the basic variable in LDFT is the single-particle density matrix γ_{ij} with respect to the sites i and j. The situation is similar to the density-matrix functional theory proposed by Gilbert for the study of nonlocal pseudopotentials[23] since the hoppings are nonlocal in the sites.

The ground-state energy E_{gs} and density matrix γ^{gs}_{ij} are determined by minimizing the energy functional

$$E[\gamma] = E_K[\gamma] + W[\gamma] \tag{2}$$

with respect to γ_{ij}. $E[\gamma]$ is defined for all density matrices that derive from a physical state, i.e., that can be written as

$$\gamma_{ij} = \sum_{\sigma} \gamma_{ij\sigma} = \sum_{\sigma} \langle \Psi | \hat{c}^{\dagger}_{i\sigma} \hat{c}_{j\sigma} | \Psi \rangle, \tag{3}$$

where $|\Psi\rangle$ is an N-particle state. Such γ_{ij} are said to be pure-state N representable. In some cases it is also useful to distinguish the subset of so-called pure-state interacting v-representable γ_{ij} or simply v-representable γ_{ij}, which are those that can be derived from a ground state of Eq. (1), i.e., $\gamma_{ij}=\gamma^{\text{gs}}_{ij}$ for some values of ε_i, t_{ij}, and U. An extension of the definition domain of $E[\gamma]$ to ensemble-representable density matrices

$$\Gamma_{ij} = \sum_{n} w_n \langle \Psi_n | \sum_{\sigma} \hat{c}^{\dagger}_{i\sigma} \hat{c}_{j\sigma} | \Psi_n \rangle, \tag{4}$$

with $w_n \geq 0$ and $\Sigma_n w_n = 1$, is straightforward following the work of Valone.[24]

The first term in Eq. (2) is given by

$$E_K[\gamma] = \sum_{i} \varepsilon_i \gamma_{ii} + \sum_{i \neq j} t_{ij} \gamma_{ij}. \tag{5}$$

It includes all single-particle contributions, namely, the crystal-field energy and the kinetic energy associated with the electron delocalization. Notice that both the diagonal and off-diagonal parts are taken into account exactly.[17]

The second term in Eq. (2) is the interaction-energy functional,

$$W[\gamma] = \min_{\Psi \to \gamma} \left[U \sum_{i} \langle \Psi[\gamma] | \hat{n}_{i\uparrow} \hat{n}_{i\downarrow} | \Psi[\gamma] \rangle \right], \tag{6}$$

which is given by Levy's constrained-search minimization.[21] Here the optimization runs over all N-particles states $|\Psi[\gamma]\rangle$ that satisfy

$$\langle \Psi[\gamma] | \sum_{\sigma} \hat{c}^{\dagger}_{i\sigma} \hat{c}_{j\sigma} | \Psi[\gamma] \rangle = \gamma_{ij} \tag{7}$$

for all i and j. Thus, $W[\gamma]$ represents the minimum possible value of the interaction energy that is compatible with a given density matrix γ_{ij}, i.e., with a given charge distribution and degree of electron delocalization. W is a universal functional of γ_{ij} in the sense that it is independent of the external parameters ε_i and t_{ij}, i.e., of the system under study. How-

ever, it depends on the number of electrons N_e, on the internal structure of the many-body Hilbert space as given by N_e and the number of orbitals or sites N_a, and on the kind of the many-body interactions in the present case Hubbard's on-site form.[10,25] It is often convenient to express W in terms of the Hartree-Fock energy E_{HF} and the correlation energy E_c as $W=E_{\mathrm{HF}}+E_c$. Notice that, in contrast to the KS approach, the expression for the kinetic, crystal-field, and exchange energies are exact, so that E_c includes only the Coulomb correlation contributions.

Finally, the variational principle for the ground-state density matrix $\gamma_{ij}^{\mathrm{gs}}$ follows from the relations[21]

$$E_{\mathrm{gs}} \leq E[\gamma] = E_K[\gamma] + W[\gamma] \tag{8}$$

for all pure-state N-representable γ_{ij} and

$$E_{\mathrm{gs}} = E_K[\gamma^{\mathrm{gs}}] + W[\gamma^{\mathrm{gs}}], \tag{9}$$

where $E_{\mathrm{gs}}=\langle\Psi_{\mathrm{gs}}|\hat{H}|\Psi_{\mathrm{gs}}\rangle$ refers to the ground-state energy.

III. COMPUTING THE EXACT INTERACTION-ENERGY FUNCTIONAL

In order to determine $W[\gamma]$ we seek the extremes of

$$F = U\sum_l (\langle\Psi|\hat{n}_{l\uparrow}\hat{n}_{l\downarrow}|\Psi\rangle) + \varepsilon(1-\langle\Psi|\Psi\rangle) + \sum_{i,j}\lambda_{ij}\left(\langle\Psi|\sum_\sigma \hat{c}_{i\sigma}^\dagger\hat{c}_{j\sigma}|\Psi\rangle - \gamma_{ij}\right) \tag{10}$$

with respect to $|\Psi\rangle$. Lagrange multipliers ε and λ_{ij} have been introduced to enforce the normalization of $|\Psi\rangle$ and the representability of γ_{ij}. Derivation with respect to $\langle\Psi|$, ε, and λ_{ij} yields the eigenvalue equations

$$\sum_{\substack{\langle ij\rangle \\ \sigma}} \lambda_{ij}\hat{c}_{i\sigma}^\dagger\hat{c}_{j\sigma}|\Psi\rangle + U\sum_i \hat{n}_{i\uparrow}\hat{n}_{i\downarrow}|\Psi\rangle = \varepsilon|\Psi\rangle \tag{11}$$

and the auxiliary conditions $\langle\Psi|\Psi\rangle=1$ and $\gamma_{ij}=\langle\Psi|\Sigma_\sigma\hat{c}_{i\sigma}^\dagger\hat{c}_{j\sigma}|\Psi\rangle$. The Lagrange multipliers λ_{ij} play the role of energy levels ($i=j$) and hopping integrals ($i\neq j$) to be chosen in order that $|\Psi\rangle$ yields the given γ_{ij}. The pure-state representability of γ_{ij} ensures that there is always a solution.

In practice, one usually varies λ_{ij} systematically in order to scan the full domain of representability of γ_{ij}. For given λ_{ij}, the eigenstate $|\Psi_0\rangle$ corresponding to the lowest eigenvalue of Eq. (11) yields the minimum $W[\gamma]$. Any other $|\Psi\rangle$ satisfying $\gamma_{ij}=\langle\Psi|\Sigma_\sigma\hat{c}_{i\sigma}^\dagger\hat{c}_{j\sigma}|\Psi\rangle$ would have higher ε and higher W since γ_{ij} and E_K are fixed. These are the so-called interacting v-representable γ_{ij}, which can be derived from a ground state of Eq. (11) or (1). They are the physically relevant ones since they necessarily include the absolute minimum $\gamma_{ij}^{\mathrm{gs}}$ of $E[\gamma]$. However, one also finds pure-state representable γ_{ij}, which correspond to excited states or to linear combinations of eigenstates of Eq. (11). Therefore, the domains of v and N representabilities are in general different, as it will be discussed below.

Equation (11) can be solved numerically for finite lattices with different structures, boundary conditions, and band fillings. In this case we expand $|\Psi[\gamma_{ij}]\rangle$ in a complete set of basis states $|\Phi_m\rangle$ which have definite occupation numbers $\nu_{i\sigma}^m$ at all orbitals $i\sigma$ ($\hat{n}_{i\sigma}|\Phi_m\rangle=\nu_{i\sigma}^m|\Phi_m\rangle$ with $\nu_{i\sigma}^m=0$ or 1). The values of $\nu_{i\sigma}^m$ satisfy the usual conservation of the number of electrons $N_e=N_{e\uparrow}+N_{e\downarrow}$ and of the z component of the total spin $S_z=(N_{e\uparrow}-N_{e\downarrow})/2$, where $N_{e\sigma}=\Sigma_i\nu_{i\sigma}^m$. For not too large clusters, the ground state $|\Psi_0[\gamma_{ij}]\rangle$ of Eq. (11) can be determined by sparse-matrix diagonalization procedures, for example, by using Lanczos iterative method.[22] Usually, $|\Psi_0[\gamma_{ij}]\rangle$ is calculated in the subspace of minimal S_z since this ensures that there are no *a priori* restrictions on the total spin S. In addition, spin-projector operators may be used to investigate the dependence of $W[\gamma]$ on S.[26]

Interesting examples of non-v-representable γ_{ij} are found when there is a discontinuous change in the nature of the ground state as a function of external or interaction parameters. Consider, for instance, the Hubbard model on a bipartite finite ring with $N_a=4k$ sites (k is a positive integer) and sublattice energy levels ε_1 and ε_2 [see Eq. (1)]. In the homogeneous case ($\Delta\varepsilon=\varepsilon_2-\varepsilon_1=0$) the Fermi energy corresponding to half-band filling is degenerate ($n=1$). This degeneracy is removed for arbitrary small values of U or $\Delta\varepsilon$. However, the nature of the ground state is completely different for $U>0$ ($\Delta\varepsilon=0$) and $\Delta\varepsilon>0$ ($U=0$). In the first case the charge distribution remains homogeneous for all $U>0$, while in the second a CDW state sets in, with a finite amplitude Δn^0 even for arbitrary small $\Delta\varepsilon$. As a result, the density matrices having $0<\gamma_{11}-\gamma_{22}<\Delta n^0$ and off-diagonal γ_{12} close to the uncorrelated limit γ_{12}^0 are not pure-state v representable. Consequently, the domain of v representability is concave. In fact, for the examples to be discussed in Sec. IV it is not simply connected since the level crossing occurs even for $U/t\to+\infty$. Notice, however, that this is a finite-size effect which tends to disappear as the length $N_a=4k$ of the ring increases. For large N_a the contribution of the Fermi level to γ_{ij} and to its discontinuity becomes negligible.

In the non-v-representable region Levy's constrained-search minimum $|\Psi_0[\gamma_{ij}]\rangle$ is given by a linear combination $|\Psi\rangle=a|\alpha\rangle+b|\beta\rangle$ of the two ground states which level crossing is at the origin of the discontinuity of $\gamma_{ij}^{\mathrm{gs}}$ ($\langle\alpha|\beta\rangle=0$). The coefficients $a>0$ and $b=\sqrt{1-a^2}e^{i\varphi}$ are obtained by minimizing $W[\gamma]$ under the constraint $\langle\Psi|\hat{c}_{i\sigma}^\dagger\hat{c}_{j\sigma}+\hat{c}_{j\sigma}^\dagger\hat{c}_{i\sigma}|\Psi\rangle=\gamma_{ij\sigma}+\gamma_{ji\sigma}$. Without loss of generality we assume that the hopping integrals are always real so that the energy functionals depends only on the sum of γ_{ij} and γ_{ji} ($t_{ij}=t_{ji}$). It is easy to see that any intermediate γ_{ij} is not pure-state v representable but it can be derived from a ket of the form $|\Psi\rangle=a|\alpha\rangle+i\sqrt{1-a^2}|\beta\rangle$. In this range the density matrix has the form $\gamma_{ij}=a^2\gamma_{ij}^\alpha+(1-a^2)\gamma_{ij}^\beta$, where γ_{ij}^α and γ_{ij}^β are the density matrices corresponding to $|\alpha\rangle$ and $|\beta\rangle$. The interaction energy associated to $|\Psi\rangle$ is $W=a^2W^\alpha+(1-a^2)W^\beta$. It necessarily yields the minimum of Levy's constrained search since $|\Psi\rangle$ is one of the ground states of the Hubbard model. Any other state representing the same γ_{ij} would have the same kinetic energy and, therefore, an equal or higher W. This shows that the N-representability domain is convex even if the v-representability domain is concave. This is an important prerequisite for the analysis of the scaling properties of $W[\gamma]$ to be performed in Sec. V.

The functional $W[\gamma]$, valid for all lattice structures, hybridizations, and energy levels, can be simplified at the ex-

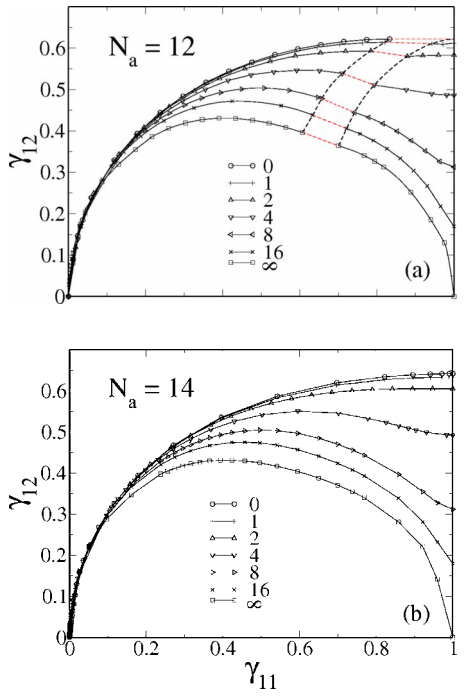

FIG. 1. (Color online) Correlation between the off-diagonal nearest-neighbor density-matrix element γ_{12} and the electron density γ_{11} at one of the sublattices of the 1D Hubbard model: (a) $N_a=12$ sites and (b) $N_a=14$ sites for half-band filling $n=(\gamma_{11}+\gamma_{22})/2=1$. Different Coulomb repulsions $U/t>0$ are considered as indicated in the inset. The dashed lines (red) indicate the γ_{ij} that are not pure-state v representable. Pure-state N representability holds for all $0\leq\gamma_{12}\leq\gamma_{12}^0$, where γ_{12}^0 refers to the $U=0$ upper bound.

pense of universality if the hopping integrals are short ranged. For example, if only NN hoppings are considered, the kinetic energy E_K is independent of the density-matrix elements between sites that are not NNs. Therefore, the constrained search in Eq. (6) may be restricted to the $|\Psi[\gamma_{ij}]\rangle$ that satisfy $\langle\Psi[\gamma_{ij}]|\Sigma_\sigma\hat{c}_{i\sigma}^\dagger\hat{c}_{j\sigma}|\Psi[\gamma_{ij}]\rangle=\gamma_{ij}$ only for $i=j$ and for NN ij. In this way the number of variables in $W[\gamma]$ is reduced significantly rendering the interpretation and practical manipulation of the functional dependence far simpler. While this is a great advantage, it also implies that W loses its universal character since the dependence on the NN γ_{ij} is in general different for different lattices. In Sec. V a number of representative exact results for $W[\gamma]$ are compared in order to quantify this behavior.

IV. REPRESENTABILITY OF THE DENSITY MATRIX

In the following we focus for simplicity on bipartite lattices choosing $\gamma_{12}>0$ and $t_{ij}=-t<0$ for NN ij. Nonbipartite lattices can be treated analogously by considering positive and negative domains of γ_{12} separately, positive (negative) values of γ_{12} being relevant for negative (positive) hopping integrals. As shown in Ref. 17 for homogeneous density distributions, nonbipartite lattices show scaling properties of $W[\gamma]$ that are similar to the bipartite case. In Fig. 1 the NN density matrix element γ_{12} of the ground state of the inhomogeneous Hubbard model is shown as a function of the electron density γ_{11} at one of the sublattices. The results refer to rings having $N_a=12$ and 14 sites and a band filling $n=N_e/N_a=1$. They were obtained from Lanczos exact diagonalizations for representative values of the Coulomb repulsion strength $U/t>0$ by varying systematically the difference $\Delta\varepsilon=\varepsilon_1-\varepsilon_2>0$ between the energy levels of the sublattices. The curves are shown only for $0\leq\gamma_{11}\leq1$ since the results are unchanged by replacing γ_{11} by $\gamma_{22}=2-\gamma_{11}$. They display the correlation between diagonal and off-diagonal elements of the density matrices γ_{ij}, as derived from the ground state of the model for different values of the parameters that define the system (i.e., the energy level difference $\Delta\varepsilon$ and the NN hopping t). These density matrices are referred to as pure-state interacting v representable or simply v representable by analogy with the DFT of the inhomogeneous electron gas. In the continuum theory the electron densities $\rho(\vec{r})$ derived from exact ground states are called interacting v representable since they stay in one-to-one correspondence with an external potential $v_{\text{ext}}(\vec{r})$.[1–3] While the v-representable domain contains all the ground-state γ_{ij}^{gs}, it is also important to investigate the properties of the more general N-representable γ_{ij}, which constitute the domain of definition of Levy's functional $W[\gamma]$.

For each γ_{11} or charge transfer $\Delta n=\gamma_{22}-\gamma_{11}$, the upper bound γ_{12}^0 for the NN γ_{12} corresponds to the largest possible value of the kinetic energy, which is achieved by the uncorrelated ground state for the given Δn. Since the underlying electronic state is a single Slater determinant, the interaction energy is given by the Hartree-Fock value $W^0=W[\gamma^0]=UN_a(\gamma_{11}^2+\gamma_{22}^2)/8$, except in cases with unusual degeneracies in the single-particle spectrum (e.g., $N_a=N_e=4$ and $\Delta n=0$). The uncorrelated γ_{12}^0 is largest for an homogeneous density distribution ($\Delta n=0$) and decreases monotonically as the charge transfer increases. It vanishes in the limit where only one sublattice is occupied (see Fig. 1). This can be understood by recalling that in an uncorrelated state an increase in Δn is the result of an increasing difference $\Delta\varepsilon$ in the energy levels of the sublattices, which reduces in its turn the possibility for the electrons to delocalize. In the limit of complete charge transfer ($\gamma_{11}\to0$) no charge fluctuations at all are possible.

For $\gamma_{12}<\gamma_{12}^0$ and a given Δn, the dimension of the subspace of accessible many-body states is larger and, therefore, the electrons can reduce the optimum value of the interaction W for a fixed γ_{ij} by reducing the number of double occupations ($U>0$). The minimum value of the interaction energy per site is $W^\infty=U(1-\gamma_{11})/2$ for $n=1$ and $\gamma_{11}\leq1$. We shall denote by γ_{12}^∞ the largest possible value of γ_{12} compatible with the minimum number of double occupations W^∞/U. γ_{12}^∞ defines the lower bound for the v representable γ_{ij} and corresponds to the ground state of the model for $U\to+\infty$ [$W(\gamma_{12}^\infty)=W^\infty$; see Fig. 1]. Smaller values of γ_{12} are still pure-state N representable. To show this one may consider a linear combination of two states having the same γ_{11} and opposite γ_{12}^∞. One of them is the ground state yielding γ_{12}^∞ for negative t_{ij} and the other for positive t_{ij} ($U\to+\infty$). It is easy to see that these states have all the same minimal interaction energy W^∞. Therefore W is independent of γ_{12} and equal to W^∞ for $|\gamma_{12}|\leq\gamma_{12}^\infty$. Although they are pure-state representable, these

γ_{ij} can never match a ground state since there are states having the same Δn and W but larger γ_{12}.

In the absence of charge transfer ($\gamma_{11}=\gamma_{22}=1$) the minimum $W^{\infty}=0$ can only be achieved by any of the 2_a^N fully localized states for which $\gamma_{12}^{\infty}=0$. This corresponds to the well-known Heisenberg limit of the homogeneous Hubbard model. However, as charge transfer increases it is possible to delocalize part of the electrons, even in the limit of strong correlations (i.e., $W=W^{\infty}$). Therefore, $\gamma_{12}^{\infty}>0$ for $0<\gamma_{11}<1$. Although the details of the strongly correlated ground state are quite complex, one can easily estimate that γ_{12}^{∞} should be larger than the γ_{12} of a Slater determinant having one localized (e.g., up) electron in the sites of the sublattice 2 ($\gamma_{22}>1$), while the remaining (e.g., down) electrons occupy delocalized states following an average occupation $\gamma_{22}-1$ on sublattice 2 and γ_{11} on sublattice 1. Consequently, γ_{12}^{∞} should be largest for intermediate values of the number of delocalized electrons per site. This corresponds roughly to a half-filled delocalized subband ($\gamma_{11}=\gamma_{22}-1\sim 1/2$ and $\Delta\varepsilon/U\sim 1$). The resulting γ_{12}^{∞} presents, therefore, a maximum as a function of γ_{11}, vanishing only for $\Delta n=1$ and $\Delta n=0$, where the number of delocalized electrons or holes is zero (see Fig. 1). Notice that the actual maximum of γ_{12}^{∞} is found for $\gamma_{11}<1/2$.

Figure 1(a) shows an interesting example of a disconnected domain of v representability, which is the result of the crossing between the two lowest $S=0$ levels. One of them favors a strong CDW state and is the ground state for large Δn, while the other yields a rather uniform density distribution and dominates for γ_{11} close to 1. The ground-state density matrix $\gamma_{ij}^{\mathrm{gs}}$ is discontinuous at the level crossing, as indicated by the dashed lines in Fig. 1(a). For $U=0$ the discontinuity appears for a arbitrary small Δn. As $U>0$ increases, $\gamma_{12}^{\mathrm{gs}}$ decreases and the transition from an homogeneous to an inhomogeneous density distribution shifts to a finite increasing $\Delta\varepsilon$. In contrast, the discontinuity in γ_{11} remains approximately constant even for $U\to+\infty$ [see Fig. 1(a)]. This leads to a whole range of γ_{ij} that cannot be attained by the ground state of the Hubbard model. Therefore, the domain of pure-state v representability is not simply connected. In this intermediate region, γ_{ij} can be represented by a linear combination of the two orthogonal degenerate ground states at the origin of the level crossing. As discussed in Sec. II, Levy's constrained-search functional W corresponds here to the interpolation of the interaction energies in the two degenerate states as given by the straight dashed lines in Fig. 1(a).

V. SCALING PROPERTIES OF INTERACTION-ENERGY FUNCTIONAL

In this section we present and discuss exact results for W in the 1D Hubbard rings that were obtained from Lanczos diagonalizations by varying systematically γ_{ij}, the band filling n, and the number of sites N_a. In Fig. 2 W is shown as a function of γ_{12} for representative values of $\Delta n=\gamma_{22}-\gamma_{11}$. Despite the strong dependence of W on Δn there are several important qualitative properties shared by all the curves:

(i) As already discussed, the domain of N representability of γ_{12} is bounded by the bond order γ_{12}^0 in the uncorrelated limit. γ_{12}^0 decreases monotonously as Δn increases vanishing for $\Delta n=2$. This is an important contribution to the Δn dependence of W, which reflects the interplay between charge transfer and electron delocalization.

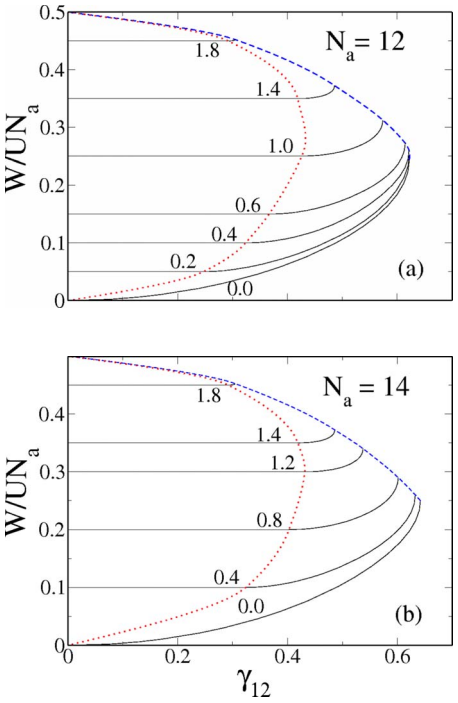

FIG. 2. (Color online) Interaction energy W of the Hubbard model on 1D rings as a function of NN density-matrix element γ_{12}: (a) $N_a=12$ and (b) $N_a=14$ sites at half-band filling $n=1$. The different charge transfers $\Delta n=\gamma_{22}-\gamma_{11}$ are indicated by the numbers labeling the curves. The dashed curve (blue) shows the Hartree-Fock upper bound $E_{\mathrm{HF}}=W^0=UN_a[n^2+(\Delta n/2)^2]/4$. The dotted curve (red) corresponds to the strongly correlated limit, where $\gamma_{12}=\gamma_{12}^{\infty}$ and $W=W^{\infty}=UN_a\Delta n/4$ for $n=1$. Notice that W is constant for $0\le\gamma_{12}\le\gamma_{12}^{\infty}$.

(ii) In the delocalized limit, $W(\gamma_{12}^0,\Delta n)=W^0=E_{\mathrm{HF}}$ for all Δn since the electronic state yielding the largest γ_{12} is a single Slater determinant. Moreover, one observes that $\partial W/\partial\gamma_{12}$ diverges at $\gamma_{12}=\gamma_{12}^0$. This is a necessary condition in order that the ground-state density matrix satisfies $\gamma_{12}^{\mathrm{gs}}<\gamma_{12}^0$ for arbitrary small $U>0$, as expected from perturbation theory.

(iii) Starting from γ_{12}^0, W decreases with decreasing γ_{12}, reaching its lowest possible value $W^{\infty}=UN_a(\gamma_{22}-1)/2$ for $\gamma_{12}=\gamma_{12}^{\infty}$ ($W^{\infty}=UN_a\Delta n/4$ for $n=1$). The decrease in W with decreasing γ_{12} means that the reduction in the Coulomb energy due to correlations is done at the expense of kinetic energy or electron delocalization. Reducing γ_{12} beyond γ_{12}^{∞} cannot lead to any further reduction in W for the given Δn.

(iv) The strongly correlated γ_{12}^{∞} is, in general, finite showing a nonmonotonous dependence on Δn. It vanishes only for $\Delta n=0$, where the electrons are localized evenly at all sites keeping just their spin degree of freedom and for $\Delta n=2$, where all the electrons form localized pairs on one sublattice. In the latter case both γ_{12}^{∞} and γ_{12}^0 vanish.

(v) In the limit of small $\gamma_{12}-\gamma_{12}^{\infty}>0$, one observes that $W\propto U(\gamma_{12}-\gamma_{12}^{\infty})^2$. Therefore, for $U/t\gg 1$, $(\gamma_{12}^{\mathrm{gs}}-\gamma_{12}^{\infty})\propto t/U$

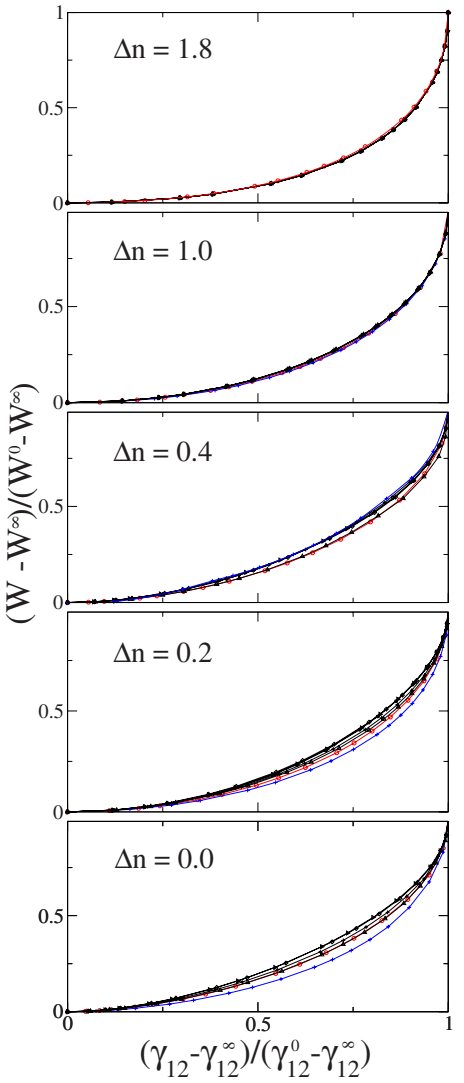

FIG. 3. (Color online) Scaled interaction energy W of the 1D Hubbard model as a function of the degree of electron delocalization $g_{12}=(\gamma_{12}-\gamma_{12}^{\infty})/(\gamma_{12}^{0}-\gamma_{12}^{\infty})$. $W^0=E_{\mathrm{HF}}$ and γ_{12}^{0} refer to the uncorrelated limit ($U=0$), while W^{∞} and γ_{12}^{∞} refer to the strongly correlated limit ($U/t\to+\infty$). Results are given for band filling $n=1$, all even numbers of sites $N_a=2-14$, and different charge transfers Δn. Open circles (red) correspond to $N_a=2$ and crosses (blue) correspond to $N_a=4$. The other sizes are very difficult to tell apart.

and $E_{\mathrm{gs}}-W^{\infty}\propto t^2/U$, results expected from perturbation theory and which correspond to the Heisenberg or t-J limit of the homogeneous Hubbard model.[7]

In order to compare the functional dependence of W for different Δn and to analyze its scaling behavior we focus on the v representable domain $\gamma_{12}^{\infty}\leq\gamma_{12}\leq\gamma_{12}^{0}$, where W is not trivially constant. To this aim it is useful to bring the domains of representability for different N_a to a common range and to scale W with respect to the Hartree-Fock and strongly correlated values. We, therefore, consider $(W-W^{\infty})/(W^0-W^{\infty})$ as a function of $g_{12}=(\gamma_{12}-\gamma_{12}^{\infty})/(\gamma_{12}^{0}-\gamma_{12}^{\infty})$ as displayed in Fig. 3 ($W^0=E_{\mathrm{HF}}$). In this form the results for different N_a appear as remarkably similar, showing that the largest part of the dependence of W on γ_{12} and Δn comes from the domain of representability of γ_{ij} and the limiting

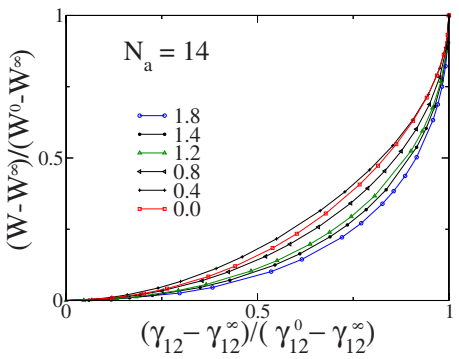

FIG. 4. (Color online) Charge transfer dependence of the scaled interaction-energy functional W of the 1D Hubbard model. Results are given as a function of the degree of electron delocalization $g_{12}=(\gamma_{12}-\gamma_{12}^{\infty})/(\gamma_{12}^{0}-\gamma_{12}^{\infty})$ for $N_a=14$, $n=1$, and different charge transfers $\Delta n=0.0-1.8$ as indicated in the inset.

values for weak and strong correlations. An analogous scaling behavior has been found in previous numerical studies of W for an homogeneous charge distribution.[17] In this case one also observes that $W(g_{12})$ depends weakly on system size N_a provided it is measured in units of the Hartree-Fock energy E_{HF} and if γ_{12} is scaled within the relevant domain of representability $[\gamma_{12}^{\infty},\gamma_{12}^{0}]$. In the present context, Fig. 3 implies that the change in W associated to a given change in the degree of delocalization g_{12} can be regarded as nearly independent of system size.

The very good scalability of W as a function of g_{12} for different system sizes is not obvious. In fact, if one considers $W(g_{12})$ for different charge transfers Δn, one observes much more significant deviations. This is demonstrated in Fig. 4 where the results for a 1D ring with $N_a=14$ sites are compared for different Δn. Qualitatively, the dependence of W on the degree of delocalization g_{12} is similar for different Δn. Notice, for instance, the behavior for weak and strong correlations ($g_{12}\approx 0$ or 1) and the overall shape in the crossover region. This shows that the scaling hypothesis works satisfactorily even for different Δn. However, the quantitative differences between the scaled W for various Δn are more significant than those found for different sizes (see Figs. 3 and 4). This is actually not very surprising since the nature of the electronic correlations is expected to evolve as we move from purely metallic to strongly ionic-like bonds. It is, therefore, important to investigate systematically the functional dependence of W for different Δn in order to elucidate its scaling behavior and evaluate the possibilities of transferring it from simple to complex many-body problems.

In Fig. 5 the band-filling dependence of W in a $N_a=10$ site Hubbard ring is shown for $N_e\leq N_a$ and $\gamma_{12}\geq 0$. The same functional dependence is obtained for $N_e>N_a$ or $\gamma_{12}<0$ due to electron-hole symmetry and the bipartite symmetry of the lattice $[W(\gamma_{12},\Delta n)=W(\pm\gamma_{12},\pm\Delta n)]$. While $W(\gamma_{12})$ depends strongly on n and Δn, several qualitative features are common to all the curves:

(i) As in the half-filled band case, the domain of v representability of γ_{12} is limited by the bond orders in the uncorrelated and strongly correlated limits: $\gamma_{12}^{0}\leq\gamma_{12}\leq\gamma_{12}^{\infty}$, where γ_{12}^{0} (γ_{12}^{∞}) corresponds to the ground state of the model for

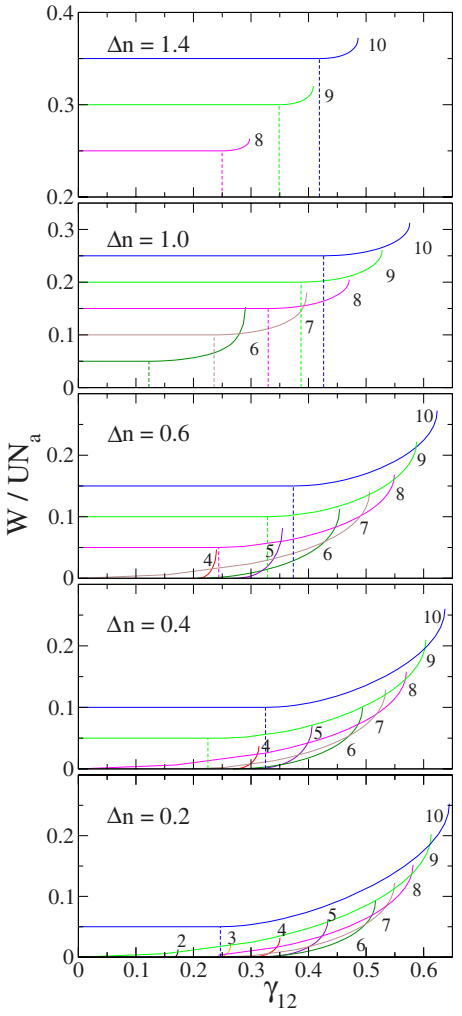

FIG. 5. (Color online) Interaction energy W of the 1D Hubbard model as a function of NN density-matrix element γ_{12} for representative charge transfers $\Delta n=\gamma_{22}-\gamma_{11}$. Results are given for $N_a=10$ sites and different band fillings $n=N_e/N_a$. The numbers indicate the number of electrons N_e corresponding to each curve and the vertical dash lines show the value of γ_{12}^{∞} below which $W=W^{\infty}$ remains constant.

$U=0$ $(U\rightarrow+\infty)$. Notice that γ_{12}^{0} increases monotonously with N_e as the single-particle band is filled up. In contrast the behavior of γ_{12}^{∞} is more complex, showing either a monotonous increase with n for $\Delta n\geq 1$ or nonmonotonous band-filling dependence for $\Delta n<1$ (see Fig. 5). As already discussed, the dependences of γ_{12}^{0} and γ_{12}^{∞} on n and Δn are of central importance to the band-filling dependence of W.

(ii) In the weakly correlated limit, $W(\gamma_{12}^{0},\Delta n)=W^{0}$ is given by the Hartree-Fock energy $E_{\mathrm{HF}}/N_a=U(n^2+\Delta n^2/4)/2$ since the underlying state is a single Slater determinant.[27] Moreover, the divergence of $\partial E_{\mathrm{C}}/\partial\gamma_{12}$ for $\gamma_{12}=\gamma_{12}^{0}$ shows that $\gamma_{12}^{\mathrm{gs}}<\gamma_{12}^{0}$ for arbitrary small $U>0$, as expected from perturbation theory.

(iii) Starting from $\gamma_{12}=\gamma_{12}^{0}$, W decreases monotonously with decreasing γ_{12}, reaching its lowest possible value $W^{\infty}=UN_a\max\{0,n-1+\Delta n/2\}/2$ for $\gamma_{12}=\gamma_{12}^{\infty}$. As already discussed for $n=1$, γ_{12}^{∞} defines the lower bound of the domain of v representability. Smaller γ_{12} are still pure-state representable but $W=W^{\infty}$ is constant in this range. For the sake of clarity, the values of γ_{12}^{∞} are indicated by vertical dashed lines. Notice that W^{∞} vanishes for small electron density, provided that the charge transfer is not very strong (i.e., $n+\Delta n/2=\gamma_{22}\leq 1$). The decrease in W with decreasing γ_{12} illustrates, once more, how the correlation-induced reduction in the Coulomb energy occurs at the expense of kinetic energy or electron delocalization.

(iv) γ_{12}^{∞} always represents the largest NN bond order that can be constructed under the constraint of minimal Coulomb repulsion energy. As in the uncorrelated case, the density-matrix element γ_{12}^{∞} vanishes when the occupation of one of the sublattices is either 0 or 2 (i.e., $\gamma_{11}=0$ under the assumption $\gamma_{11}<\gamma_{22}$ and $n\leq 1$). However, in the strongly correlated limit, γ_{12}^{∞} also vanishes when the occupation of one of the sublattices is strictly 1 since this leaves no possibility for the electrons or holes to delocalize without involving charge fluctuations (bipartite lattice). This is of course only possible for $n\geq 1/2$. One, therefore, finds, assuming $\gamma_{11}<\gamma_{22}$, that $\gamma_{12}^{\infty}=0$ for $\gamma_{22}=n+\Delta n/2=1$.

(v) For small n or Δn, where both γ_{11} and γ_{22} are smaller than 1, it is possible to approximate the strongly correlated state (minimal W) by a fully polarized Nagaoka state as in the homogeneous case.[18] In this case γ_{12}^{∞} is largest for $\Delta n=0$, decreasing monotonously with increasing Δn, and vanishing for $\gamma_{11}=0$ $(\Delta n=n)$ or $\gamma_{22}=1$ $[\Delta n=2(1-n)]$ whichever comes first. This explains the nonmonotonous dependence of γ_{12}^{∞} as a function of n with a maximum for $n=1/2$ for $\Delta n<1$ (i.e., nearly half-filled fully polarized spin band).

(vi) In the other regime, for $\Delta n>1$ $[1/2<n<1$ and $\gamma_{22}=(n+\Delta n/2)>1]$ one can obtain a lower bound for γ_{12}^{∞} by assuming localized electrons in sublattice 2, for instance, with spin up, so that γ_{12} is given by the remaining $N_e-N_a/2$ down electrons. While this ansatz neglects spin fluctuations and is, therefore, rather poor quantitatively, it explains the monotonous increase in γ_{12}^{∞} with increasing n for fixed $\Delta n>1$ as the down band is filled up (see Fig. 5). The approximation remains qualitatively correct provided that $\gamma_{22}=(n+\Delta n/2)>1$. In particular it explains that γ_{12}^{∞} vanishes for $\gamma_{11}=0$ and $\gamma_{22}=1$ and that, for a given n, it shows a local maximum for Δn not far from 1 $[2(1-n)\leq\Delta n\leq 2n]$, i.e., for $\gamma_{11}\simeq\gamma_{22}-1$, when the delocalized electrons are evenly distributed among the two sublattices (see Fig. 5, for example, for $N_e=8$).

The results for different band fillings are compared in Fig. 6 by considering the scaled interaction energy $(W-W^{\infty})/(W^{0}-W^{\infty})$ as a function of $g_{12}=(\gamma_{12}-\gamma_{12}^{\infty})/(\gamma_{12}^{0}-\gamma_{12}^{\infty})$. Once the relevant v-representable domains are brought to a common range, one observes a remarkably similar behavior for all band fillings. Figure 6 shows that the largest part of the band-filling dependence of W in the inhomogeneous Hubbard model comes from its limiting values $W^{0}=E_{\mathrm{HF}}=UN_a(n^2+\Delta n^2/4)/2$ and $W^{\infty}=UN_a\max\{0,n-1+\Delta n/2\}/2$ and on the corresponding bounds γ_{12}^{0} and γ_{12}^{∞} of the domain of representability. Similar conclusions are inferred from calculations for other sizes and lattice structures. Notice that the strongest dependence of the scaled interaction on n is found for a nearly homogeneous charge density (small Δn) and for intermediate values of g_{12}. As we approach the strongly correlated limit $(g_{12}\leq 0.4)$ the dependence of n is relatively

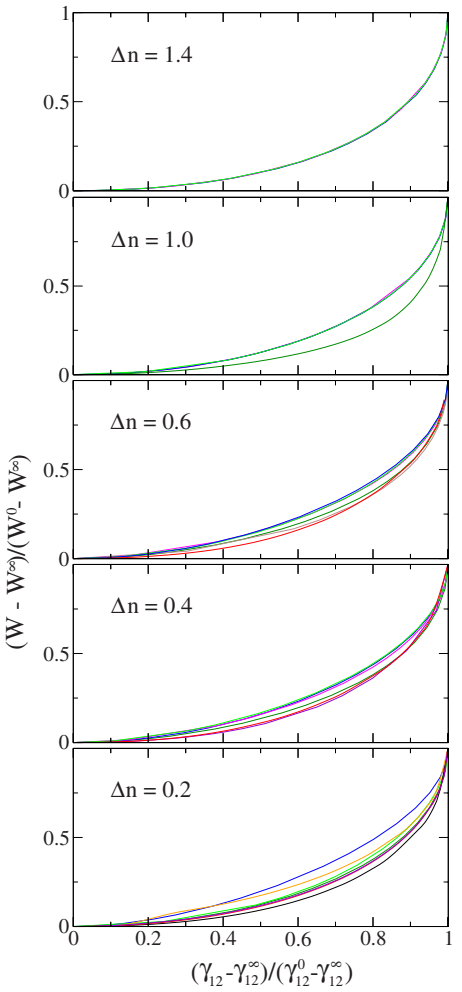

FIG. 6. (Color online) Scaled interaction energy of the 1D Hubbard model for $N_a=10$ sites as a function of $g_{12}=(\gamma_{12}-\gamma_{12}^{\infty})/(\gamma_{12}^{0}-\gamma_{12}^{\infty})$. For each charge transfer Δn results are given for different band fillings $n=N_e/N_a$ as in Fig. 5.

weak even for $\Delta n \simeq 0$. One concludes that a properly scaled interaction energy follows approximately a universal behavior.

VI. SUMMARY AND OUTLOOK

A density-functional approach to lattice-fermion models has been applied to the inhomogeneous Hubbard model. In the framework of lattice density-functional theory (LDFT) the basic variable is the single-particle density matrix γ_{ij} and the central functional is the interaction energy $W[\gamma]$. The challenge is, therefore, to determine $W[\gamma]$ and to provide with useful accurate approximations for it. In this paper we have presented a systematic study of the functional dependence of W of the Hubbard model as a function the NN density-matrix element γ_{12} and charge transfer $\Delta n=\gamma_{22}-\gamma_{11}$. Rigorous numerical results have been obtained from exact Lanczos diagonalizations on finite supercells with periodic boundary conditions. The functional dependence of W has been analyzed by varying the degree of charge transfer and electron delocalization between the sublattices, as well as the number of sites N_a and the band filling $n=N_e/N_a$. It has been shown that W can be appropriately scaled as a function of Δn and $g_{12}=(\gamma_{12}-\gamma_{12}^{\infty})/(\gamma_{12}^{0}-\gamma_{12}^{\infty})$, where γ_{12}^{0} (γ_{12}^{∞}) refers to the limit of weak (strong) electronic correlations. In other words, the change in W associated with a given change in the degree of NN charge transfer and electron delocalization can be regarded as nearly independent of the system under study.

The observed pseudouniversal behavior of the scaled interaction energy functional provides a unified description of correlations from weak- to strong-coupling regimes. Moreover, it encourages transferring the results from supercells to infinite systems with different lattice geometries. In this way the scope of LDFT has been extended to inhomogeneous charge-density distributions. A basis for applications to more realistic lattice models in low symmetry configurations is thereby provided. Among the interesting perspectives one can mention multileg ladders including the crossover to the two-dimensional square lattice, metal clusters, and disordered systems. Furthermore, it would be relevant to apply the present scaling approximation to other types of interactions. For instance, in the attractive Hubbard model the nature of the electronic correlations and the resulting properties of the functional $W[\gamma]$ are fundamentally different. The same holds for the conditions for v representability of γ_{ij}, which depend on the explicit form of the Hamiltonian, in contrast to the notion of N representability which involves the whole Hilbert space of the system and only depends on the number of sites and electrons. For $U<0$, W corresponds to the maximum number of double occupations for a given γ_{ij}. Therefore, new interesting effects are expected, particularly concerning the interplay between homogeneous and inhomogeneous density distributions.

ACKNOWLEDGMENT

Computer resources provided by the Computer Center of the University of Kassel are gratefully acknowledged.

[1] P. Hohenberg and W. Kohn, Phys. Rev. **136**, B864 (1964).
[2] R. G. Parr and W. Yang, *Density-Functional Theory of Atoms and Molecules* (Clarendon, Oxford, 1989).
[3] R. M. Dreizler and E. K. U. Gross, *Density Functional Theory* (Springer, Berlin, 1990), and references therein.
[4] W. Kohn and L. J. Sham, Phys. Rev. **140**, A1133 (1965).
[5] U. von Barth and L. Hedin, J. Phys. C **5**, 1629 (1972).
[6] D. C. Langreth and M. J. Mehl, Phys. Rev. B **28**, 1809 (1983); A. D. Becke, Phys. Rev. A **38**, 3098 (1988); J. P. Perdew, K. Burke, and M. Ernzerhof, Phys. Rev. Lett. **77**, 3865 (1996), and references therein.
[7] See, for instance, P. Fulde, *Electron Correlations in Molecules*

and Solids (Springer, Berlin, 1991); N. H. March, *Electron Correlation in Molecules and Condensed Phases* (Plenum, New York, 1996); G. D. Mahan, *Many-Particle Physics* (Kluwer, New York, 2000).

[8] E. Dagotto, Rev. Mod. Phys. **66**, 763 (1994); A. Georges, G. Kotliar, W. Krauth, and M. J. Rozenberg, *ibid.* **68**, 13 (1996); M. Imada, A. Fujimori, and Y. Tokura, *ibid.* **70**, 1039 (1998).

[9] P. W. Anderson, Phys. Rev. **124**, 41 (1961).

[10] J. Hubbard, Proc. R. Soc. London, Ser. A **276**, 238 (1963); J. Kanamori, Prog. Theor. Phys. **30**, 275 (1963); M. C. Gutzwiller, Phys. Rev. Lett. **10**, 159 (1963).

[11] R. Pariser and R. G. Parr, J. Chem. Phys. **21**, 466 (1953); **21**, 767 (1953); J. A. Pople, Trans. Faraday Soc. **49**, 1375 (1953).

[12] O. Gunnarsson and K. Schönhammer, Phys. Rev. Lett. **56**, 1968 (1986); A. Svane and O. Gunnarsson, Phys. Rev. B **37**, 9919 (1988); K. Schönhammer, O. Gunnarsson, and R. M. Noack, *ibid.* **52**, 2504 (1995).

[13] A. Schindlmayr and R. W. Godby, Phys. Rev. B **51**, 10427 (1995).

[14] A. E. Carlsson, Phys. Rev. B **56**, 12058 (1997); R. G. Hennig and A. E. Carlsson, *ibid.* **63**, 115116 (2001).

[15] N. A. Lima, M. F. Silva, L. N. Oliveira, and K. Capelle, Phys. Rev. Lett. **90**, 146402 (2003).

[16] C. Verdozzi, Phys. Rev. Lett. **101**, 166401 (2008).

[17] R. López-Sandoval and G. M. Pastor, Phys. Rev. B **61**, 1764 (2000).

[18] R. López-Sandoval and G. M. Pastor, Phys. Rev. B **66**, 155118 (2002).

[19] R. López-Sandoval and G. M. Pastor, Phys. Rev. B **67**, 035115 (2003).

[20] R. López-Sandoval and G. M. Pastor, Phys. Rev. B **69**, 085101 (2004).

[21] M. Levy, Proc. Natl. Acad. Sci. U.S.A. **76**, 6062 (1979).

[22] C. Lanczos, J. Res. Natl. Bur. Stand. **45**, 255 (1950); B. N. Parlett, *The Symmetric Eigenvalue Problem* (Prentice-Hall, Englewood Cliffs, 1980).

[23] T. L. Gilbert, Phys. Rev. B **12**, 2111 (1975); For more recent studies see, for example, S. Goedecker and C. J. Umrigar, Phys. Rev. Lett. **81**, 866 (1998), and references therein.

[24] S. M. Valone, J. Chem. Phys. **73**, 1344 (1980); **73**, 4653 (1980).

[25] The LDFT formalism can be easily extended to arbitrary interactions $H_I=(1/2)\Sigma V_{ijkl}\hat{c}^{\dagger}_{i\sigma}\hat{c}^{\dagger}_{k\sigma'}\hat{c}_{l\sigma'}\hat{c}_{j\sigma}$ by replacing $U\Sigma_i\hat{n}_{i\uparrow}\hat{n}_{i\downarrow}$ by H_I in the expressions for the interaction-energy functional $W[\gamma]$. However, note that the functional dependence of W on γ depends crucially on the form of V_{ijkl} (see also Refs. 17 and 19).

[26] R. López-Sandoval and G. M. Pastor (unpublished).

[27] In the presence of degeneracies in the single-particle spectrum one may find that Levy's minimum W does not derive from a single Slater determinant and that $W^0 < E_{\mathrm{HF}}$. However, this is a finite-size effect whose importance decreases with increasing N_a.