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Electronic properties of strongly correlated fermions in nanostructures

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Abstract

Lattice density-functional theory is applied to small clusters described by the Hubbard model in order to study the effect of the correlation on these nano-objects. Results for the ground-state energy and charge excitation gap of small clusters are presented and discussed as a function of the number of sites N_a , Coulomb repulsion U/t , and band filling n .

1. Introduction

Clusters are currently studied in two different contexts in solid-state physics. On the one hand, they are used as models for calculating properties of infinite systems which are local in nature or which can be approximated by a discrete sampling in k space [1]. In this framework the *finite size* of the cluster is a limitation of which the consequences must be minimized, for example, by performing finite-size scaling analysis. On the other hand, in recent years it has become possible to produce isolated clusters containing a small number of atoms as well as cluster-based nanostructures on surfaces and to study their properties experimentally in various ways [2]. For these atomic clusters the characteristic physical behaviours resulting from the limited dimensions of the sample and from the large surface-to-volume ratio are the central issue.

Electron correlations in finite systems and the associated many-body phenomena which distinguish small particles from atoms and solids are a subject of main concern in current cluster research. In this paper, several ground-state properties of one-dimensional (1D) clusters are investigated by using a recently developed lattice density-functional theory (LDFT) of strongly correlated fermions [3–5]. The systems are described in the framework of the Hubbard Hamiltonian [6], which, together with related models, has been successfully applied in past years to the study of the low-energy electronic properties of various nanostructures and low-dimensional materials (for example, clusters [7], fullerene molecules [8], polymeric chains [9], two-dimensional (2D) lattices [10], etc).

The remainder of the paper is organized as follows. In section 2, the main steps of the LDFT formulation are briefly recalled. Explicit approximations to the interaction-energy functional W of the Hubbard model are presented in section 3. Results for the ground-state energy and charge excitation gap of finite rings and cagelike 12-atom clusters are discussed in section 4. Finally, some perspectives of future research directions are pointed out.

2. Density-functional theory of lattice fermion models

In order to be explicit we focus on the Hubbard model [6] which is expected to capture the main physics of lattice fermions in a narrow energy band. The Hamiltonian

$$H = \sum_{(i,j)\sigma} t_{ij} \hat{c}_{i\sigma}^\dagger \hat{c}_{j\sigma} + U \sum_i \hat{n}_{i\downarrow} \hat{n}_{i\uparrow}, \quad (1)$$

includes nearest neighbour (NN) hoppings t_{ij} , and on-site interactions given by U ($\hat{n}_{i\sigma} = \hat{c}_{i\sigma}^\dagger \hat{c}_{i\sigma}$). The hopping integrals t_{ij} are defined by the lattice structure and by 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} . The situation is similar to the density-matrix functional theory proposed by Gilbert for the study of nonlocal pseudopotentials [11], since the hoppings are nonlocal in the sites. A formulation of DFT on a lattice in terms of the diagonal γ_{ii} alone is possible only if one restricts oneself to models with constant t_{ij} for $i \neq j$ [12].

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

$$E[\gamma] = E_{\text{K}}[\gamma] + W[\gamma] \quad (2)$$

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

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

where $|\Psi\rangle$ is an N -particle state. Such γ_{ij} are said to be pure-state N -representable. An extension of the definition domain of E to ensemble-representable density matrices Γ_{ij} is straightforward following the work by Valone [13]. The first term in equation (2) is the kinetic energy associated with the electronic motion in the lattice. It is given by

$$E_{\text{K}}[\gamma] = \sum_{ij} t_{ij} \gamma_{ij}, \quad (4)$$

thus including all single-particle contributions. The second term is the interaction-energy functional given by

$$W[\gamma] = \min_{\Psi \rightarrow \gamma} \left[U \sum_i \langle \Psi[\gamma] | \hat{n}_{i\uparrow} \hat{n}_{i\downarrow} | \Psi[\gamma] \rangle \right], \quad (5)$$

where the minimization runs over all N -particle states $|\Psi[\gamma]\rangle$ that satisfy

$$\langle \Psi[\gamma] | \sum_{\sigma} \hat{c}_{i\sigma}^\dagger \hat{c}_{j\sigma} | \Psi[\gamma] \rangle = \gamma_{ij} \quad (6)$$

for all i and j [14]. $W[\gamma]$ represents the minimum value of the interaction energy compatible with a given density matrix γ_{ij} . It is a universal functional of γ_{ij} in the sense that it is independent of t_{ij} , i.e., of the system under study. Nevertheless, W depends on the number of electrons N_e , on the structure of the many-body Hilbert space, as given by N_e and the number of

orbitals or sites N_a , and on the form of the interaction Hamiltonian. The LDFT formalism can be readily extended to arbitrary interactions $H_I = (1/2) \sum V_{ijkl} \hat{c}_{i\sigma}^\dagger \hat{c}_{k\sigma}^\dagger \hat{c}_{l\sigma} \hat{c}_{j\sigma}$, by replacing $\sum_i \hat{n}_{i\uparrow} \hat{n}_{i\downarrow}$ by H_I in $W[\gamma]$. However, notice that such a general functional depends crucially on the considered model interaction as given by the form of V_{ijkl} .

$E[\gamma]$ is minimized by expressing

$$\gamma_{ij} = \sum_{\sigma} \gamma_{ij\sigma} = \sum_{k\sigma} u_{ik\sigma} \eta_{k\sigma} u_{jk\sigma}^* \quad (7)$$

in terms of the eigenvalues $\eta_{k\sigma}$ (occupation numbers) and eigenvectors $u_{ik\sigma}$ (natural orbitals) of $\gamma_{ij\sigma}$. Lagrange multipliers μ and $\lambda_{k\sigma}$ ($\varepsilon_{k\sigma} = \lambda_{k\sigma} / \eta_{k\sigma}$) are introduced in order to impose the constraints $\sum_{k\sigma} \eta_{k\sigma} = N_e$ and $\sum_i |u_{ik\sigma}|^2 = 1$. Deriving with respect to $u_{jk\sigma}^*$ and $\eta_{k\sigma}$ ($0 \leq \eta_{k\sigma} \leq 1$), one obtains the eigenvalue equations

$$\eta_{k\sigma} \sum_i \left(t_{ij} + \frac{\partial W}{\partial \gamma_{ij}} \right) u_{ik\sigma} = \varepsilon_{k\sigma} u_{jk\sigma}, \quad (8)$$

with the subsidiary conditions $\varepsilon_{k\sigma} < \mu$ if $\eta_{k\sigma} = 1$, $\varepsilon_{k\sigma} = \mu$ if $0 < \eta_{k\sigma} < 1$, and $\varepsilon_{k\sigma} > \mu$ if $\eta_{k\sigma} = 0$ [3, 11]. Self-consistency is implied by the dependence of $\partial W / \partial \gamma_{ij}$ on $\eta_{k\sigma}$ and $u_{ik\sigma}$. This formulation is analogous to density-matrix functional theory in the continuum [11]. However, it differs from KS-like approaches which assume non-interacting v -representability and where only integer occupations are allowed [12, 15–17]. In the present case, the fractional occupations of natural orbitals play a central role. One may in fact show that in general $0 < \eta_{k\sigma} < 1$ for all $k\sigma$. Exceptions are found only in very special situations like the uncorrelated limit ($U = 0$) or the fully polarized ferromagnetic state in the Hubbard model ($S_z = \min\{N_e, 2N_a - N_e\}/2$). This can be understood from perturbation-theory arguments, since none of the $\eta_{k\sigma}$ is a good quantum number for $U \neq 0$, and is explicitly verified by exact solutions of the Hubbard Hamiltonian on finite systems or the 1D infinite chain [18]. The non-integer occupation of all natural orbitals implies that the eigenvalues $\varepsilon_{k\sigma}$ in equation (8) must be degenerate. Consequently, the ground-state density matrix satisfies

$$t_{ij} + \frac{\partial W}{\partial \gamma_{ij}} = \delta_{ij} \mu. \quad (9)$$

Notice the importance of the dependence of W on the off-diagonal density-matrix elements γ_{ij} which measure the degree of electron delocalization. Approximations of W in terms of the diagonal γ_{ii} alone are not applicable in this framework ($t_{ij} \neq 0$ for NN ij). Equation (9) provides a formal scheme to solve for the ground-state γ_{ij}^{gs} according to the variational principle. For practical applications one needs of course explicit approximations to $W[\gamma]$ providing an accurate description of the electronic properties of the model in different interaction regimes, band-fillings, and lattice structures. This is discussed in the following section.

3. Interaction-energy functionals for the Hubbard model

The general functional $W[\gamma]$, valid for all lattice structures and for all types of hybridization, can be simplified at the expense 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 equation (5) may be restricted to the $|\Psi[\gamma]\rangle$ that satisfy equation (6) only for $i = j$ and for NN ij . This reduces significantly the number of variables in $W[\gamma]$ and renders the determination and interpretation of the functional dependence far simpler. In particular for periodic lattices, symmetry considerations require that all NN density-matrix elements of the ground state have the same value, i.e., $\gamma_{ij} = \gamma_{12}$ for all NN pairs ij . Therefore, the interaction-energy functional

W can be regarded as a simple function of the NN density-matrix element γ_{12} . Notice, however, that in this way W loses its universal character, since the NN map and the resulting dependence of W on γ_{12} are in principle different for different kinds of lattice [3].

In order to derive simple approximations to $W(\gamma_{12})$, one may take advantage of some general properties, in particular of the scaling behaviour of $W(\gamma_{12})$ within its domain of representability [3, 4]. Exact numerical studies [3] have in fact shown that $W(\gamma_{12})$ depends weakly on N_e , N_a and lattice structure if it is measured in units of the Hartree–Fock energy E_{HF} and if γ_{12} is scaled within the relevant domain of representability $[\gamma_{12}^\infty, \gamma_{12}^0]$. Here γ_{12}^∞ represents the largest NN bond order that can be obtained under the constraint of vanishing Coulomb energy, and γ_{12}^0 is the largest representable value of γ_{12} corresponding to the maximum degree of electron delocalization. In other words, the relative change in W associated with a change in the degree of delocalization

$$g_{12} = (\gamma_{12} - \gamma_{12}^\infty)/(\gamma_{12}^0 - \gamma_{12}^\infty) \quad (10)$$

can be approximated as nearly independent of the system under study. The functional dependence of W on g_{12} can then be extracted from a simple reference system. Using the exact analytical result for the Hubbard dimer, one obtains the dimer or second-order approximation $W^{(2)}$ which reads [4]

$$W^{(2)}(\gamma_{12}) = E_{\text{HF}} \left(1 - \sqrt{1 - g_{12}^2} \right). \quad (11)$$

Notice that E_{HF} , γ_{12}^∞ and γ_{12}^0 are system specific. In practice, γ_{12}^∞ may be approximated by the ferromagnetic fully polarized γ_{12}^{FM} which is derived, like E_{HF} and γ_{12}^0 , from the solution of the single-particle spectrum. Equation (11) has been previously applied to determine several ground-state properties of 1D, 2D, and 3D systems in the thermodynamical limit [4]. In particular, for the infinite 1D chain, it has been shown that the LDFT results for the ground-state energy E_{gs} are remarkably close to the exact Bethe ansatz solution for all band fillings n . For $n \leq 0.8$ the LDFT results are nearly indistinguishable from the exact ones. Even the largest discrepancies, found for $n = 1$ and intermediate U/t , are acceptably small (i.e., of the order of 10%). However, for $n = 1$ and $U/t \gg t$, equation (11) yields $E_{\text{gs}} \simeq -\alpha_2 t^2/U$ with $\alpha_2 \simeq 3.24$, while the exact result is $\alpha_{\text{ex}} = 4 \ln 2 \simeq 2.77$. In order to overcome this shortcoming in the case of strong correlations, a more flexible functional has been introduced, which includes a fourth-order term in g_{12} . In this case the interaction energy takes the form

$$W^{(4)} = E_{\text{HF}} \left(1 - \sqrt{1 - \kappa g_{12}^2 + (\kappa - 1) g_{12}^4} \right), \quad (12)$$

where $\kappa = \alpha_{\text{ex}}/\alpha_2 > 0$ is the ratio between the small- γ_{12} expansion coefficients of W^{ex} and $W^{(2)}$. The value of κ depends somewhat on the lattice structure or system dimensions. At half band filling it can be determined by applying perturbation theory to the Heisenberg limit of the Hubbard model [19]. For instance, for the 1D chain one obtains $\kappa_{1\text{D}} = 8/(\pi^2 \ln 2) = 1.169$. Notice that $\kappa_{1\text{D}}$ is not very far from the dimer value $\kappa = 1$, for which equation (12) reduces to equation (11). Therefore, the fourth-order term appears as a relatively small correction to the second-order approximation. Equation (12) provides a systematic improvement at half band filling for all values of the interaction strength U/t . In the following section equations (11) and (12) are applied in the framework of LDFT to determine several electronic properties of the Hubbard model on finite clusters.

4. Results and discussion

In figure 1 results are given for the ground-state energy E_{gs} of 1D Hubbard rings as a function of number of sites N_a for representative values of the Coulomb interaction U/t and band

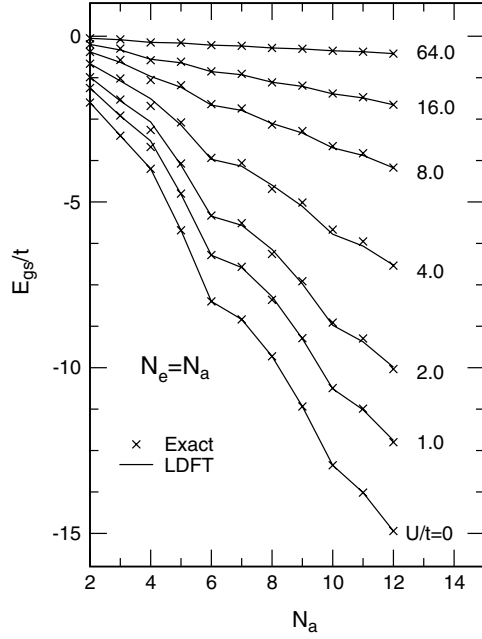


Figure 1. Ground-state energy of Hubbard rings as a function of the number of sites N_a for half band filling $n = N_e/N_a = 1$ and different values of the Coulomb repulsion U/t . The crosses refer to exact diagonalization results obtained using the Lanczos method. The lines are a guide to the eye connecting the results of lattice density-functional theory (LDFT).

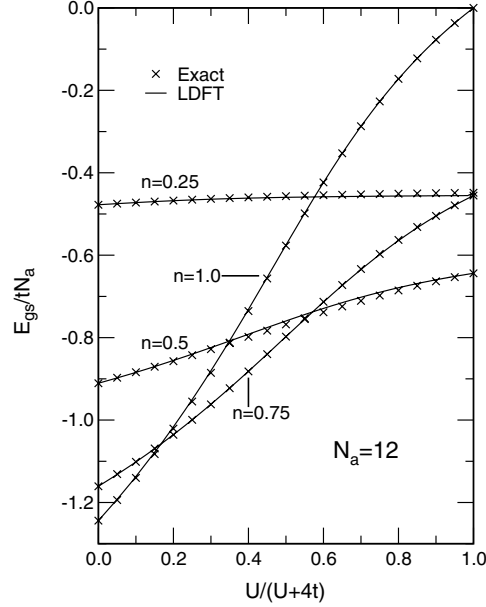


Figure 2. Ground-state energy of a Hubbard ring with $N_a = 12$ sites as a function of the Coulomb repulsion U/t for different band fillings $n = N_e/N_a$. The crosses refer to exact diagonalization results obtained using the Lanczos method and the curves to lattice density functional theory (LDFT).

filling $n = N_e/N_a = 1$. The LDFT calculations are compared with exact numerical results obtained by using the Lanczos method [20]. One observes that LDFT yields very good results for all ring sizes and interaction regimes. For weak and strong interactions ($U/t \leq 1$ and $U/t \geq 16$) the LDFT values are extremely close to the exact ones, while for intermediate interaction strengths (e.g., $U/t = 4$) some minor discrepancies are appreciable. In all cases the trends as a function of cluster size N_a are very well reproduced (see figure 1). In order to investigate the changes in the ground-state properties for different band fillings, we present in figure 2 results for E_{gs} as a function of U/t for a periodic ring with $N_a = 12$ sites and $n = 1/4, 1/2, 3/4$, and 1. On one side, E_{gs} increases monotonically with U/t with a slope $\partial E_{\text{gs}}/\partial U = \sum_i \langle n_{i\uparrow} n_{i\downarrow} \rangle > 0$ that is smaller for smaller density. On the other side, for small U/t , E_{gs} decreases with increasing n as the single-particle band is filled ($n \leq 1$). As a result, a non-monotonic band-filling dependence is observed in the limit of strong correlations. This behaviour is very well reproduced by LDFT for all band fillings and interaction regimes (see figure 2). The very good performance holds not only for E_{gs} but also for the separate kinetic and Coulomb contributions, which implies that electron localization and intra-atomic correlations are correctly described for all U/t . Therefore, the accuracy obtained for the ground-state energy is not the consequence of a compensation of errors. It is also interesting to observe that in the present LDFT calculations no artificial symmetry breaking is required in order to describe correlation-induced localization correctly, as it is often the case in other approaches, for example, in a mean-field spin density-wave state in the unrestricted Hartree–Fock approximation [8] or in the saddle-point slave boson method [21]. Moreover, the LDFT

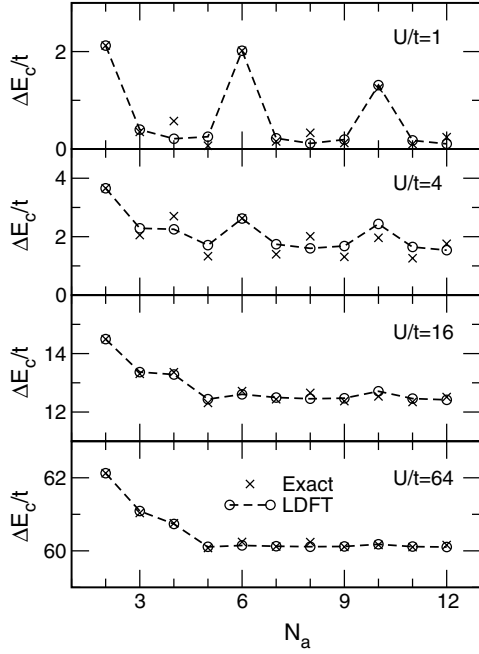


Figure 3. Charge excitation gap ΔE_c of Hubbard rings as a function of the number of sites N_a for different values of the Coulomb repulsion U/t . The crosses refer to exact diagonalization results obtained using the Lanczos method. The open circles connected by dashed lines are the results of lattice density-functional theory (LDFT).

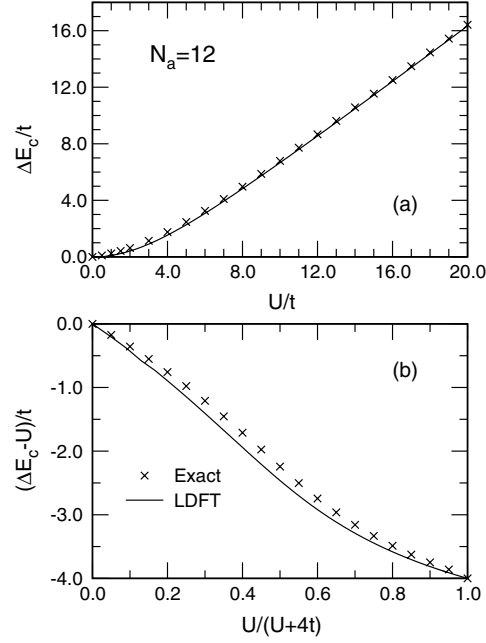


Figure 4. Charge excitation gap ΔE_c of a Hubbard ring with $N_a = 12$ sites as a function of U/t . The solid curves refer to LDFT and the symbols to exact numerical diagonalizations [20].

calculations remain simple and numerically not demanding, since the minimization of E_{gs} involves analytical expressions for E_K and W (see equations (4), (11), and (12)). One concludes that LDFT, combined with equations (11) and (12) as approximations to the interaction-energy functional, provides an accurate description of ground-state electron correlations in finite 1D rings.

The charge excitation gap or bandgap defined by

$$\Delta E_c = E_{gs}(N_e + 1) + E_{gs}(N_e - 1) - 2E_{gs}(N_e) \quad (13)$$

is a property of considerable interest in strongly correlated systems. In the thermodynamic limit it can be related to the discontinuity in the derivative of the kinetic and correlation energies per site with respect to the electronic density n . Thus, the determination of ΔE_c constitutes a much more serious challenge than the calculation of ground state properties, particularly in the framework of a density-functional formalism. In figure 3 results are shown for ΔE_c of Hubbard rings as a function of the number of sites N_a for representative values of U/t . For small U/t one observes oscillations of ΔE_c as a function of N_a which are related to the structure of the single-particle spectra of the rings. These are progressively attenuated as U/t increases and finally disappear in the strongly interacting limit. Consequently, the convergence to the infinite chain limit is faster for large U/t . Concerning the comparison between LDFT and exact results, one observes, as in the case of E_{gs} , that our method performs at its best for weak and strong interactions. However, even in the crossover regime, e.g., $U/t = 4$, the quantitative discrepancies are fairly small and the overall trends are well reproduced. The dependence of

ΔE_c on U/t is shown in figure 4 for the case of a 12-site ring. ΔE_c increases with increasing U/t ($\Delta E_c = 0$ for $U/t = 0$) and approaches the limit $\Delta E_c \rightarrow (U - w_b)$ for $U/t \rightarrow \infty$, where w_b is the width of the single-particle band of the 1D ring. Comparison between LDFT and exact results shows a good overall agreement. It should however be noted that the gap is somewhat underestimated for $U/t \ll 1$. Nevertheless, the accuracy of LDFT improves rapidly with increasing U/t , as electron localization starts to set in. The error in ΔE_c tends to zero for large U/t , and therefore the development of a Mott-insulator-like state is correctly described.

Calculations have also been performed for cage-like or fullerene Hubbard clusters in order to explore the effects of lattice frustrations on the ground-state properties. In the case of the icosahedral C_{12} structure, the LDFT results have been compared with exact and unrestricted Hartree–Fock (UHF) calculations. LDFT gives in general a much better description of ground-state energy E_{gs} as a function of n and U/t than UHF. For example, in the intermediate and strongly interacting regimes UHF overestimates E_{gs} significantly while the differences between the exact and LDFT results are very small. This reflects limitations of the broken symmetry UHF solutions, even in the most general non-collinear case [8]. Let us recall that no symmetry breakings are required in LDFT in order to correctly reproduce these correlation effects. Moreover, the charge excitation gaps obtained in this framework are in good agreement with exact diagonalizations. Therefore, one expects that LDFT should be an efficient tool for investigating the properties of larger fullerenes such as C_{20} , C_{60} , and C_{70} which are inaccessible to exact diagonalization methods. In this way the available UHF studies [8] could be significantly improved. Research in this direction is currently in progress.

In summary, a novel lattice density functional approach to electron correlations in lattice models has been applied to the determination of several electronic properties of finite Hubbard clusters. Results for the ground-state energy and charge excitation gap of 1D rings and the icosahedral-cage C_{12} cluster demonstrate the ability of lattice density-functional theory to describe quantitatively the subtle competition between kinetic charge fluctuations and correlation induced localization. Besides the interest of these specific systems, the accuracy of the results and the simplicity of the calculations encourage further applications to the problem of electron correlations in nanostructures.

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