Extended Hubbard model with renormalized Wannier wave functions in the correlated state: beyond the parametrized models

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Abstract. The method used earlier for analysis of correlated nanoscopic systems is extended to infinite (periodic) s-band-like systems described by the Hubbard model. The optimized single-particle Wannier wave functions contained in the parameters of the extended Hubbard model (in the nearest-neighbor hopping (−t), in the magnitude of the intraatomic interaction U, and in other parameters) are determined explicitly in the correlated state for the electronic systems of various symmetries and dimensions: Hubbard chain, square and triangular planar lattices, and the three cubic lattices (SC, BCC, FCC). In effect, the evolution of the electronic properties as a function of interatomic distance R is obtained. The model parameters in most cases do not scale linearly with the lattice spacing and hence, their solution as a function of microscopic parameters reflects only qualitatively the system evolution. Also, the atomic energy changes with R and therefore should be included in the model analysis. The solutions in one dimension (D = 1) can be analyzed both rigorously (by making use of the Lieb–Wu solution) and compared with the approximate Gutzwiller treatments. In higher dimensions (D = 2 and 3) only the latter approach is possible to implement within the scheme. The renormalized single particle wave functions are almost independent of the choice of the scheme selected to diagonalize the Hamiltonian in the Fock space in D = 1 case. For dimensions D > 1 the qualitative behavior is independent of the structure considered. The wave-function size increases above the Mott-Hubbard localization threshold and gradually reaches the atomic limit value. The method can be extended to other approximation schemes, as stressed at the end.

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1 Introduction

The question of combining in an explicit manner inter-electronic correlations with single-particle (band) calculations is very important for the systems for which Coulomb interaction between electrons is comparable to or even larger than the kinetic (bare band) energy of electrons [1,2]. With respect to this, methods starting from band calculations, such as LDA+U [3] or LDA+DMFT [4] have been devised and they work well for quite few systems. The methods provide e.g. the photoemission spectrum [5], the overall band splitting at the Fermi surface (i.e. the stability of the Mott insulating state) optical spectrum, etc. The band structure calculations allow also for estimation of the Hubbard-interaction parameter U, when the Wannier functions are determined first [6]. In all these methods the question of counting twice the electron-electron Coulomb extended interaction arises when the effective single-particle potential contains them. Also, those methods do not work well in the case of low-dimensional systems.

A systematic approach relies on taking into account Coulomb interactions leading to strong correlations in an exact (or approximate) manner first and only then determining the renormalized single-particle wave functions contained in the model parameters by a proper Euler variational procedure. In that situation we allow for a readjustment of single-particle wave functions in the correlated-electron state, as well as calculate them explicitly. Such a reverse method called EDABI (Exact Diagonalization with Ab Initio Approach) has been devised and employed to nanoscopic chains and clusters [7]. It provides the evolution of the correlated-system properties as a function of interatomic distance R, not only as a function of model parameters. For example [8], EDABI provides new results such as e.g. a systematic evolution of the statistical distribution function as a function of
increasing $R$ (from Fermi-like function to a continuous momentum distribution reflecting electron localization on parent atoms) or a magnetic Slater-like splitting of the electronic states without the appearance of long-range antiferromagnetic ordering [7]. Needless to say that this method avoids in an explicit manner the double counting of the interaction between the particles. Such a reverse order of calculating the electronic states is particularly appealing for nanoscopic and low-dimensional systems, since the screening processes of the repulsive Coulomb interaction are ineffective.

The purpose of this paper is to generalize and test the EDABI-type approach for extended systems of arbitrary dimension ($D = 1, 2, 3$) described by the (parametrized) extended Hubbard model. Only in the $D = 1$ case it is possible to compare an exact (Lieb–Wu, LW) solution with the Gutzwiller-ansatz (GA) solutions. In other words, the approximate Gutzwiller-wave-functions (GWF), and the single-particle basis optimization (i.e. in the Schrödinger representation) the first and the second quantization schemes, we calculate the single-particle properties starting from the single-particle basis first and only then readjust the basis to the method selected to diagonalize the many-particle Hamiltonian in the Fock space. In general, our method of approach completes the solution of the parametrized models in the sense that it yields the evolution of the correlated many-particle systems properties as a function of interatomic distance, as well as provides the shape of the Wannier functions in the correlated state.

The structure of the paper is as follows. In Section 2 and 3 we overview briefly our method, whereas in Section 4 the extended Hubbard-chain properties are analysed in detail. In Sections 5 and 6 selected two- and three-dimensional lattices are considered, respectively. Section 7 contains a brief summary and an overview. In the Appendices A and B we provide some formal details of the calculations.

2 Parameterized models supplemented with the single-particle basis optimization a posteriori: a brief summary of EDABI

Before placing our work in the literature of the subject, we first characterize the essence of our approach [7] from the formal side. The method of the optimized single-particle wave functions incorporates the first and the second quantization schemes. Namely, if $\Psi(r_1, ..., r_N)$ describes the $N$-particle wave function in the Schrödinger representation (i.e. in the Hilbert space), then in the second-quantization representation (i.e. in the Fock space) this state can be represented by $|\Phi\rangle$

$$|\Phi\rangle = \frac{1}{\sqrt{N!}} \int d^3r_1...d^3r_N \Psi(r_1, ..., r_N)|\Psi^\dagger (r_1)...\Psi^\dagger (r_N)\rangle |0\rangle,$$

where, $\Psi^\dagger (r_1) = \left(\Psi^\dagger (r_1)\Psi^\dagger (r_1)\right)$, denotes the field operators representing the particle creation at point $r_1$ with spin $\sigma = \uparrow, \downarrow \equiv \pm 1$. Utilizing the anticommutation relations for the field operators one can easily find the inverse representation, in which the $N$-particle wave function has the form

$$\Psi(r_1, ..., r_N) = \frac{1}{\sqrt{N!}} \langle 0 | \Psi(r_1)...\Psi(r_N) |\Phi\rangle.$$

So, the two schemes are equivalent if only the anticommutation relations of the field operators are defined. Here, the field operator is defined in the single-particle basis of Wannier functions $w_i(r)$ as follows

$$\hat{\Psi}(r) = \sum_{i=1}^\infty w_i(r) a_i^\dagger,$$

where in what follows we set $M = N$ and the single-particle basis $\{w_i(r)\}$ is the single-particle-Wannier-function basis (to be defined explicitly later). In effect, the approximate states in the Fock space are defined through

$$|\Phi\rangle \approx \frac{1}{\sqrt{N!}} \sum_{j_1...j_N=1}^M C_{j_1...j_N} a_{j_1}^\dagger ...a_{j_N}^\dagger |0\rangle,$$

and the $N$-particle wave function in this approximate basis has now the form

$$\Psi(r_1, ..., r_N) = \frac{1}{\sqrt{N!}} \sum_{i_1...i_N=1}^M \sum_{j_1...j_N}^M \langle 0 | a_{i_N}...a_{i_1} a_{j_N}^\dagger ...a_{j_1}^\dagger |0\rangle \times C_{j_1...j_N} w_{i_1}(r_1)...w_{i_N}(r_N).$$

The coefficients $C_{j_1...j_N}$ can be calculated by either direct Hamiltonian diagonalization or by Lanczos method for finite systems [10], whereas the normalized (optimized) wave functions $\{w_i(r)\}$ are determined by the procedure described below. Note that the second-quantization formalism separates the many-particle function aspect of the problem, which is contained in the coefficients $C_{j_1...j_N}$, from the single-particle wave-mechanics aspect of determining the basis $\{w_i(r)\}$. In fact, the two are intertwined. Namely, we perform the diagonalization of the second-quantized Hamiltonian for selected (and fixed) single-particle basis first and only then readjust the basis $\{w_i(r)\}$ with the help of a variational approach. In many cases involving exact diagonalization for nanoscopic systems [7] the basis is readjusted in the iterative manner after each consecutive diagonalization procedure in the Fock space until the minimum energy is reached.