Correlated Electron Systems of Different Dimensionalities

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The optimized single-particle wave functions contained in the parameters of the Hubbard model (hopping integral \( t \) and intraatomic interaction \( U \)) are determined explicitly in the correlated state for electronic systems of various symmetries and dimensions: Hubbard chain, square and triangular lattices, and the three cubic lattices: SC, BCC, and FCC. In effect, the electronic properties of these structures as a function of the interatomic distance \( R \) are obtained. In most cases, the model parameters do not scale linearly with the lattice constant. Also, the atomic part of the total ground state energy changes with the \( U/t \) ratio and therefore should (and is) included in the analysis. The solutions of dimensions \( D > 1 \) are analyzed by utilizing the approximate Gutzwiller treatment.

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1. Introduction

We extended the method (exact diagonalization combined with the \textit{ab initio} approach, EDABI) used earlier for analysis of correlated nanoscopic systems [1–5] to infinite (periodic) \( s \)-band-like systems described by the Hubbard model and its extensions. We describe correlated electron systems of different dimensionalities and symmetries by using the extended Hubbard Hamiltonian

\[
H = \varepsilon_a \sum_i c_i^\dagger c_i + \sum_{(ij)\sigma} t_{ij} c_i^{\dagger} \sigma c_j \sigma + U \sum_i n_{i\uparrow} n_{i\downarrow},
\]

where \( t_{ij} \) — the hopping integral between the sites \( i \) and \( j \), \( U \) is the magnitude of the Coulomb interaction at given site \( i \), and

(175)
\[ \varepsilon_{a}^{\text{eff}} \equiv \varepsilon_a + \frac{1}{N} \sum_{i<j} \left( K_{ij} + \frac{2}{R_{ij}} \right) \]  

(2)

is the effective atomic energy reducing to the true atomic energy \( \varepsilon_a \) in the limit of large interatomic separation (\( K_{ij} \) is the corresponding quantity for electrons located on sites \( i \) and \( j \neq i \)). This energy is important in view of the fact that we will study the system evolution as a function of the interatomic distance \( R \). In that situation \( \varepsilon_{a}^{\text{eff}} \) is not a constant quality, as would be in the case for a parametrized model, but reduces to the atomic energy of the hydrogenic atom in the \( R \to \infty \) limit.

In order to determine the ground state energy we use the Gutzwiller ansatz [6] (see also [7] where we used the exact Lieb–Wu solution as well as the Gutzwiller wave function approximation (GA) for the Hubbard chain)

\[ \frac{E_G}{N} \equiv \varepsilon_{a}^{\text{eff}} - |\varepsilon| (1 - U/U_c)^2, \quad U_c = 8|\varepsilon|, \]  

(3)

where \( \varepsilon \) is the average kinetic energy of noninteracting electrons.

The formula represents a final step in solving model in GA scheme. Here, it represents a starting point in obtaining the optimized single-particle wave functions \( \{w_i(r)\} \). We construct the single-particle wave functions \( \{w_i(r)\} \) entering the expressions for \( t, U, \varepsilon_{a}^{\text{eff}}, \) and \( K_{ij} \) in the following manner:

\[ w_i(r) \equiv \beta \Psi_i(r) - \gamma \sum_{j=1}^{z} \Psi_j(r), \]  

(4)

where \( z \) is the number of nearest neighbors, \( \beta \) and \( \gamma \) are the mixing coefficients, and

\[ \Psi_i(r) \equiv \sqrt{\frac{\alpha^3}{\pi}} e^{-\alpha |r-R_i|} \]  

(5)

is the 1s-like atomic wave function centered around the site \( i \). In concrete calculations they are represented by the Gaussians from the STO-3G basis. The parameters \( \beta \) and \( \gamma \) are selected to fulfill the orthogonality of the basis. We optimized the single-particle wave function by changing the \( \alpha \) parameter in order to achieve the global minimum of the ground state energy for all interatomic distances under consideration.

2. Results and discussion

In Fig. 1 we display the ground state energy as a function of interatomic distance for Hubbard chain (CH), square (SQ) and triangular (TR) lattices. We see the \( U/t \) ratio similar for CH and SQ (cf. inset). Figure 2 shows the ground state energy and the \( U/t \) ratio as a function of interatomic distance for cubic lattices. In Fig. 3 we display the band \( (-E_B = -8d(1-2d)|\varepsilon|) \) and interaction \( (E_{\text{int}} = Ud) \) energies near critical interatomic distance for all lattices under consideration. One can see that \( -E_B \cong E_{\text{int}} \) near critical interatomic distance. Moreover, we see that the metal–insulator (Mott) transition (MIT) for a square lattice is located almost
In the same point as that for a triangular lattice. Cubic lattices have also very similar critical distances.

In summary, we determined mean-field (Gutzwiller ansatz) MIT boundaries for lattices of different dimensionality and symmetry.
Fig. 3. The band ($-E_B$) and interaction ($E_{int}$) energies near critical interatomic distance. The solid points mark the critical distances for MIT.

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References