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 be (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 *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

$$H = \varepsilon_a^{\text{eff}} + \sum_{\langle ij \rangle \sigma} t_{ij} c_{i\sigma}^\dagger c_{j\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow}, \tag{1}$$

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

$$\varepsilon_a^{\text{eff}} \overset{\text{a.u.}}{\equiv} \varepsilon_a + \frac{1}{N} \sum_{i<j} \left(K_{ij} + \frac{2}{R_{ij}} \right) \tag{2}$$

is the effective atomic energy reducing to the true atomic energy ε_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)

$$\frac{E_{\text{G}}}{N} \equiv \varepsilon_a^{\text{eff}} - |\bar{\varepsilon}| \left(1 - U/U_{\text{c}} \right)^2, \qquad U_{\text{c}} = 8|\bar{\varepsilon}|, \tag{3}$$

where $\bar{\varepsilon}$ 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 $\{w_i(\boldsymbol{r})\}$. We construct the single-particle wave functions $\{w_i(\boldsymbol{r})\}$ entering the expressions for t, U, $\varepsilon_a^{\text{eff}}$, and K_{ij} in the following manner:

$$w_i(\boldsymbol{r}) \equiv \beta\,\Psi_i(\boldsymbol{r}) - \gamma \sum_{j=1}^{z} \Psi_j(\boldsymbol{r}), \tag{4}$$

where z is the number of nearest neighbors, β and γ are the mixing coefficients, and

$$\Psi_i(\boldsymbol{r}) \equiv \sqrt{\frac{\alpha^3}{\pi}} \text{e}^{-\alpha|\boldsymbol{r}-\boldsymbol{R}_i|} \tag{5}$$

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 β and γ are selected to fulfill the orthogonality of the basis. We optimized the single-particle wave function by changing the α 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 ($-E_{\text{B}} = -8d(1-2d)|\bar{\varepsilon}|$) and interaction ($E_{\text{int}} = Ud$) energies near critical interatomic distance for all lattices under consideration. One can see that $-E_{\text{B}} \cong E_{\text{int}}$ near critical interatomic distance. Moreover, we see that the metal–insulator (Mott) transition (MIT) for a square lattice is located almost
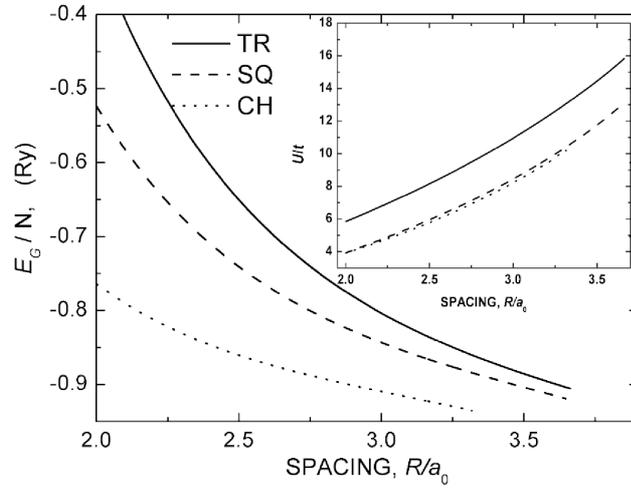
Fig. 1.   The ground state energy vs. R for CH, SQ, and TR lattices for the Gutzwiller ansatz. Inset: U/t ratio as a function of lattice parameter.
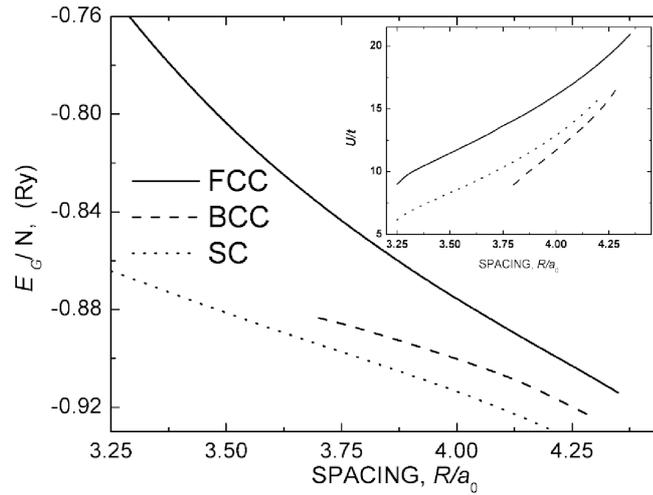

Fig. 2.   The ground state energy vs. R for SC, BCC and FCC lattices for the Gutzwiller ansatz. Inset: U/t ratio as a function of lattice parameter.

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.
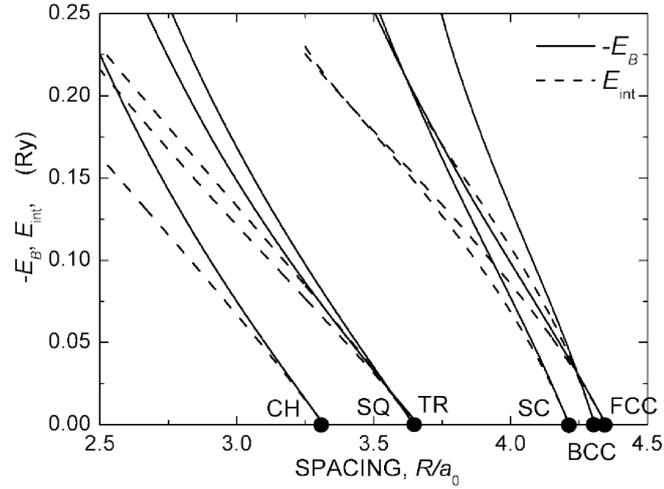
Fig. 3. The band $(-E_{\mathrm{B}})$ and interaction (E_{int}) energies near critical interatomic distance. The solid points mark the critical distances for MIT.

Acknowledgments

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