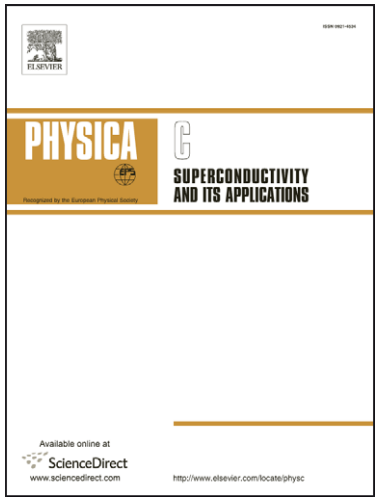

Analytical solution of extended Hubbard models on three- and four-site clusters

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Analytical solution of extended Hubbard models on three- and four-site clusters

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Abstract

The thermodynamical potential of Hubbard models extended by either nearest-neighbour Coulomb correlation and/or nearest-neighbour Heisenberg exchange is calculated analytically for a triangle and tetrahedron. It is shown that the various degeneracies of the grand-canonical energy levels are partially lifted by the exchange interaction and completely by the Falicov term. The influence of the additional interactions on the specific heat has been calculated for the tetrahedron.

Key words: Hubbard model, analytical solution, nearest-neighbour interaction, cluster
PACS: 85.80.+n, 73.22.-f, 71.27.+a

Besides the fact that the analytical solution of non-trivial models of strong correlation is a task of high pedagogical value, the renewed interest in the analytical solution stems mainly from cluster methods, which were successfully developed within the context of strong electron correlation during the last decade [1,2] and applied to problems of high-T_c superconductivity and from modelling of electron transport through quantum dots [3]. Both topics have in common that a detailed knowledge of the cluster physics is a key ingredient. The by far most employed model of strong correlated electrons is the Hubbard model. Despite its simplicity, the only analytical solutions available up to now are the groundstate for n-site rings by help of the Bethe ansatz or transfer matrix method [4,5] and the complete solution on small clusters, i.e. the triangle, the tetrahedron [6] and the square [7]. For models containing five and more sites only approximate or numerically solutions exist. One of the main points in [7] was the discovery of the degeneracy of cluster states with different particle numbers and spin, which has surely a great influence of the coupling of spin- and charge degrees of freedom. This point of view got support very recently [8,9]. Usually the addition of further terms to the pure Hubbard hamiltonian destroys this degeneracy and makes the system unsolvable due to a reduced number of symmetries. In the present paper we study the influence of nearest-neighbour (nn) Coulomb interaction $\mathbf{H}_F = W\sum_{n.n.}\mathbf{n}_i\mathbf{n}_j$, exchange term (in the case of triangle or tetrahedron) $\mathbf{H}_X = J\sum_{n.n.}\boldsymbol{S}_i\boldsymbol{S}_j$ or next-nearest neighbour (nnn) hopping $\mathbf{H}_{nnn} = t'\sum_{nnn}(\mathbf{c}^+_{i\sigma}\mathbf{c}_{j\sigma} + h.c.)$ (in the case of the square) respectively, which are added to the standard Hubbard model. Here we use the notation of Ref. [7]. For the square geometry any of the additional terms reduces the symmetry, what prevents an analytical solution. Furthermore, nnn-hopping creates frustration, what becomes evident since for $t' = t$ the model is equivalent to the pure Hubbard model on the tetrahedron. Nevertheless, there exist non-trivial parameter sets, where analytical solutions exist. Since for the triangular and tetrahedral geometry the spatial and spin symmetries are enough to get a complete solution we restrict, due to the lack of space, the considerations to those cases. Regarding the method of calculating the eigenvalues and eigenvectors we refer to [6,7]. In the following the nn-hopping parameter t is used as energy unit. For the on-site Coulomb energy $U = 4t$ was chosen, and the applied magnetic field in z-direction was set to zero, if not otherwise mentioned.

In Fig. 1 we show the electron number in dependence on the chemical potential for both the triangle and the tetrahedron respectively. For the triangle the most interesting occupation number is $N = 1$, since for the related chemical potential the empty state is degenerated both with a magnetic state with $N = 1$ and a non-magnetic state of $N = 2$. Nearest neighbour-Coulomb interaction lifts the degeneracy, whereas the exchange term does not. For the tetrahedron we find the empty state degenerated with the groundstate for $N = 1$, $N = 2$ and $N = 3$. This degeneracy is lifted partially

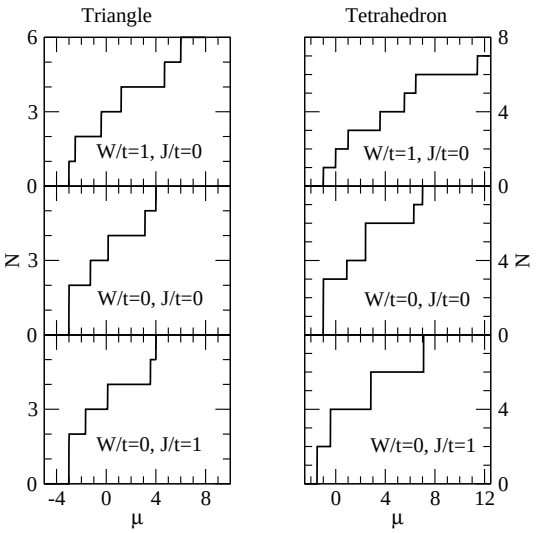

Fig. 1. $N(\mu)$ for the triangle and the tetrahedron.

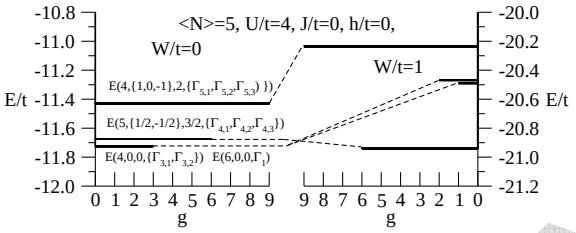

Fig. 2. The lowest energy levels for $\langle N\rangle = 5$ for the Hubbard model without (left) and with (right) nn-Coulomb interaction (Falicov term) on a tetrahedron.

by the exchange term and completely by the nnn-Coulomb interaction. Furthermore the groundstates of $N = 4$, $N = 6$ are degenerated at the related chemical potential. The benefit from formation of a spin singlet overcomes the increase of the Coulomb energy, induced by an additional electron. In Figs. 2 and 3 the influence of nn-Coulomb correlation and spin exchange on the lowest (grand-canonical) energy levels is depicted for the most interesting cases $\langle N\rangle = 5$ and $\langle N\rangle = 2$ respectively. The levels are classified by the quantum numbers of electron occupation N, spin S_z, $\vec{S}^2$, and the partners of irreducible representations of the point group T_d [6] respectively, e.g. $E(N, S_z, S(S+1), \Gamma_{m,i}$. For the "undoped" model, i.e. $\langle N\rangle = 4$, the two Γ_3-spin-singlets are the groundstates (see appendix) and the first exited states are the 9 triplet states belonging to Γ_5 and $S = 1$.

As an example of the influence of these level crossings on physical quantities, the specific heat of a cluster gas was calculated. The results for the most interesting occupation numbers are depicted in Fig. 4.

Summarising we can say, that the physics of the Hubbard model on a triangle and tetrahedron is dominated by the degeneration of groundstates belonging to different occupation numbers. The latter is lifted partially by an additional Heisenberg exchange and totally by a n.n.-Coulomb interaction.

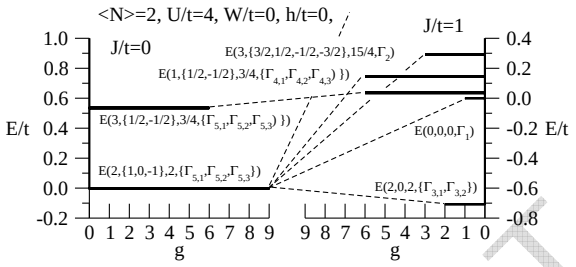

Fig. 3. The lowest energy levels for $\langle N(\mu)\rangle = 2$ for the Hubbard model without (left) and with (right) nn-Heisenberg interaction on a tetrahedron.

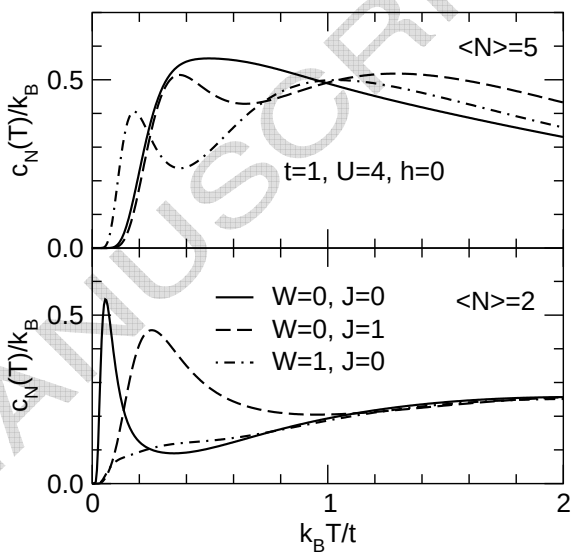

Fig. 4. The specific heat at constant electron occupation for extended Hubbard models on a tetrahedron for $< N >= 2$ and $< N >= 5$.

Appendix A. E_G on a tetrahedron for N=4

$$E(4,0,0,\{\Gamma_{3,1},\Gamma_{3,2}\}) = -J - 4\,\mu + U + 5\,W - 2\,X\,Y$$
$$Y = \cos(\arccos(4\,t^2\,(J + U - W)\,/X^3)/3)$$
$$X = \sqrt{J^2 + 16\,t^2 + 2\,J\,U + U^2 - 2\,J\,W - 2\,U\,W + W^2}/\sqrt{3}$$

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