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LETTER TO THE EDITOR

The asymmetric Hubbard model on a two-dimensional cluster

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Abstract. An interaction between two heavy electrons mediated by two light electrons is investigated within the asymmetric Hubbard model on a square cluster with 6×6 sites. The pair correlation function describing the probabilities of all relative positions of the heavy electrons is calculated by an approximative method. An effective attraction is found to exist in a certain range of model parameters.

Electrons moving among localized particles, and interacting with them locally, effectively produce an interaction between the particles. In general, this is a many-body, long-range interaction which brings about an arrangement of the localized particles, as was found, for example, for the Falicov–Kimball model (FKM) [1–4]. The FKM describes itinerant electrons that jump on a lattice, and ions fixed at the lattice sites. It is assumed here that any site may be occupied by no more than one electron and one ion. The Hamiltonian is

$$H_{\mathrm{FKM}} = -\sum_{\langle k,l\rangle} d_k^+ d_l + U \sum_k d_k^+ d_k f_k^+ f_k \tag{1}$$

where d_k and f_k are annihilation operators for the electrons and the ions, respectively, at sites $k = 1, \ldots, N$. The hopping term of the electrons is summed over all nearest-neighbour (n.n.) lattice sites $\langle k, l\rangle$ and the hopping integral is taken to be the unit of energy. The on-site interaction between ions and electrons can be either attractive ($U < 0$) or repulsive ($U > 0$). Both cases are related because of the symmetry of the Hamiltonian (1) [3].

In this letter we restrict ourselves to the repulsive case, where the ions mimic localized f electrons, and the itinerant electrons correspond to band d electrons as, e.g., in some rare-earth compounds [5]. Since in the FKM the ions do not move, the occupation number $n_k = f_k^+ f_k$ is fixed ($n_k = 0$ or 1) for every site k, and the H_{FKM} depends parametrically on the ionic configuration $\{n_k\}$. For a given N-site cluster containing N_i ions there are $\binom{N}{N_i}$ ionic configurations. It appears that the character of an effective interaction between the ions described by the FKM can be either repulsive or attractive, depending on U and electron and ion densities [4, 6]. It is natural to expect that an effective interaction between the ions will also persist after they start to move. Indeed, our previous studies of the ground-state properties of the model performed on one-dimensional clusters confirm this conjecture [7].

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Here we extend our studies to a two-dimensional cluster. The Hamiltonian that we use contains the ionic hopping term in addition to the FKM, i.e.

$$H = H_{\mathrm{FKM}} - t \sum_{\langle k,l \rangle} f_k^+ f_l \tag{2}$$

where t is the ionic hopping integral between n.n. sites $\langle k, l \rangle$. The model described by equation (2) is usually called the *asymmetric* Hubbard model (AHM), since it is a generalization of the one-band Hubbard model, allowing the hopping integrals of electrons with up and down spin to be different [8]. Indeed, the standard Hubbard model is obtained from equation (2) after putting $t = 1$, whereas $t = 0$ gives the FKM. Note that the itinerant ions can also be viewed as 'heavy electrons', since they repel the electrons ($U > 0$), and their kinetic energy is smaller than that of the electrons ($t < 1$). The effective interaction between two ions is well described by the ion–ion correlation function L:

$$L(x) = \frac{1}{N} \langle 0| \sum_{|k-l|=x} n_k n_l \, |0\rangle \tag{3}$$

where $|0\rangle$ is the ground state of the system and x denotes the distance between the sites. In order to calculate L we use a lattice version of the Born–Oppenheimer approximation (BOA), which allows us to study many-body effects at $T = 0$ for larger systems than those attainable by exact diagonalization [7]. The method consists in replacing the true ground state $|0\rangle$ by an approximate one $|0\rangle_{\mathrm{BOA}}$. This is carried out in two steps.

First, the lowest-energy states are found for every distribution $\{n_k\}$ of the N_i ions over N sites. In other words, the ground states $|\{n_k\}\rangle_0$ of the FKM Hamiltonian (1) are found for every ion configuration $\{n_k\}$ by solving the equations

$$H_{\mathrm{FKM}} |\{n_k\}\rangle_0 = \epsilon_0(\{n_k\}) |\{n_k\}\rangle_0 \tag{4}$$

where $\epsilon_0(\{n_k\})$ is the ground-state energy of the FKM corresponding to the fixed ionic configuration $\{n_k\}$. Then the functions $|\{n_k\}\rangle_0$ are chosen to form a reduced basis for the Hamiltonian H of equation (2) and all the matrix elements $\langle \{n_k\}|H|\{n_l\}\rangle$ are computed. This latter matrix is then diagonalized, and its lowest energy eigenvalue E_0 and the associated eigenvector

$$|0\rangle_{\mathrm{BOA}} = \sum_{\{n_k\}} a^0_{\{n_k\}} |\{n_k\}\rangle_0 \tag{5}$$

are used to calculate L. The method just described is believed to be relevant when the kinetic energy of the ions is much smaller than that of the electrons, i.e. for $0 < t \ll 1$, and it becomes exact for $t = 0$. We have already used the method for studying the ground-state properties of the AHM on 1d clusters [7].

Here we report the study of the effective interactions between two ions, as mediated by two electrons on a square cluster with $N = 6 \times 6$ sites, where periodic boundary conditions were imposed.

In the $t = 0$ case, i.e., with the FKM, for positive values of U it appears that the minimum energy of the system is attained when the ions are located on neighbouring lattice sites. This means that they effectively attract each other. An example of the dependence of the ground-state energy E_0 on the position of one ion when the other occupies the origin of the coordinate system is shown in figure 1 for $U = 10$.

If the ions are allowed to move ($t > 0$), then the effective interaction between them is represented by L. We found that L increases with the distance between the ions, which corresponds to an effective repulsion between them when t is not too small and U not too large. However, for sufficiently large U and small t the function decreases with distance.

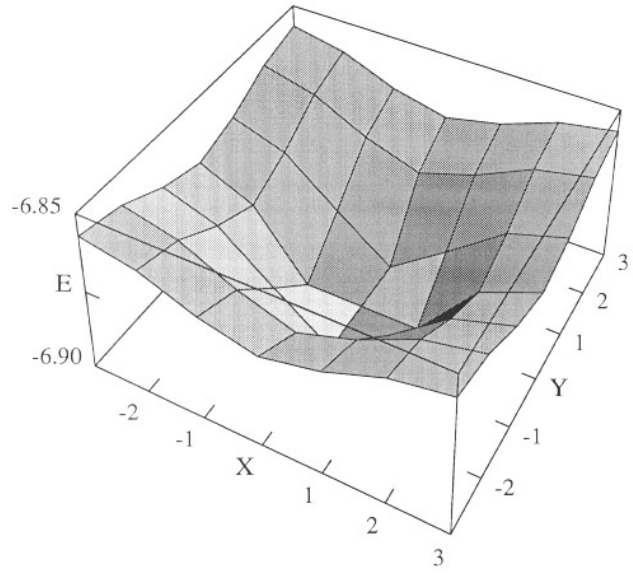

Figure 1. The ground-state energy of the FKM as a function of the distance between heavy electrons for the system of two heavy and two light electrons on a square cluster of 6×6 sites. The on-site repulsion energy is $U = 10$.

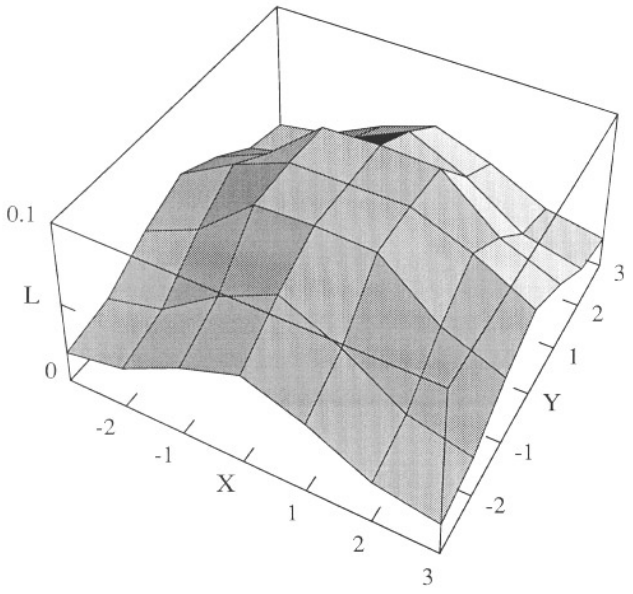

Figure 2. The pair correlation function L as a function of the distance between heavy electrons for the system of two heavy and two light electrons on a square cluster of 6×6 sites. The on-site repulsion energy is $U = 10$ and the heavy-electron hopping parameter is $t = 0.01$.

This is evidence of effective attraction between the ions (or rather between heavy electrons). Our findings are illustrated in figures 2 and 3, where L is displayed for some values of the

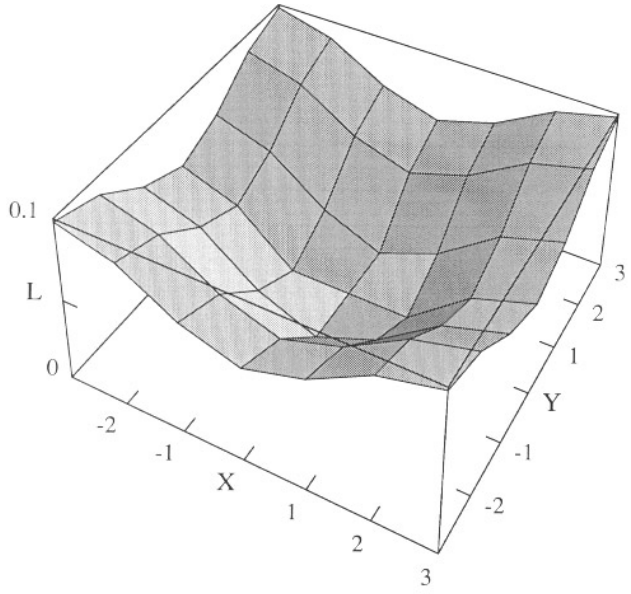

Figure 3. The same as figure 2 but with $t = 0.1$. A similar form of L is observed for smaller U (of the order of 1).

model parameters, $U = 10, t = 0.01$ and $U = 10, t = 0.1$, respectively.

The conclusions are similar to those obtained for the one-dimensional case [7]. In a purely electronic system (without phonons) an effective *attraction* between heavy electrons can be produced as a result of correlation effects. For sufficiently large positive U and sufficiently small t, heavy electrons attract each other (see figure 2), whereas for larger t or smaller U there is an effective repulsion (see figure 3) as was also found in the case of the Hubbard model ($t = 1$) [9]. In fact, the character of the interaction between the ions depends on their density as well as on the density of the electrons which mediate the interaction. However, the numerical analysis of the more general situation is severely impeded by the rapid increase of basis states, even if one uses an approximate method such as that reported here.

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