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Bounds for the Hubbard Model Free Energy: Numeric Aspects

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Abstract: In the paper [1], series of upper bounds and two lower ones for the partition function of the Hubbard model have been derived. The numerical values of upper and lower approximants have also been calculated for small systems for $U > 0$ case. Here the numeric examination of bounds is continued: the temperature behaviour of approximants is studied and the $U < 0$ case is considered.

Key words: Hubbard model, Falicov-Kimball model, exact diagonalization study

I. INTRODUCTION

In this paper, the free energy of the Hubbard model is studied. The Hubbard Hamiltonian can be written as [2]

$$H_{\text{Hub}}(t,U) = -t \sum_{\langle i,j\rangle;\sigma=\pm} \left(c_{i,\sigma}^{\dagger} c_{j,\sigma} + \text{h.c.}\right) + U \sum_{i} n_{i,+} n_{i,-} \quad (1)$$

where: i, j are site indices; we assume that all sites form a finite subset of $\mathbb{Z}^d$. t is the *hopping constant* and U is the *Coulomb interaction constant.* $c_{i,\sigma}^{\dagger}$ $\left(c_{i,\sigma}\right)$ are creation (annihilation) operators for fermion with spin σ on the i-th site; $n_{i,\sigma} = c_{i,\sigma}^{\dagger} c_{i,\sigma}$ is the particle number operator.

In the paper [1], rigorous upper and lower bounds for partition functions of the Hubbard model have been derived. These upper and lower bounds are expressible by certain objects related to corresponding Falicov-Kimball models [3, 4] (partition functions and eigenvectors).

The Hamiltonian of the *Falicov-Kimball model* with mobile particles "+" and immobile particles "–" is

$$F_{\text{FK},+}(t,U) = -t \sum_{\langle i,j\rangle} \left(c_{i,+}^{\dagger} c_{j,+} + \text{h.c.}\right) + U \sum_{i} n_{i,+} n_{i,-} \quad (2)$$

Analogically, $H_{FK,-}$ is a Hamiltonian of the FKM with "–" being mobile particles and "+" being immobile ones.

In [1], the numerical precision of these bounds has been examined for small systems. In the present paper we continue the numeric examination of upper and lower bounds. Our aim is two-fold: we examine the bounds in larger region of temperatures, and we explore the model with $U < 0$.

II. SUMMARY OF PREVIOUS RESULTS FOR UPPER AND LOWER BOUNDS

The upper and lower bounds for the partition functions of the Hubbard model are expressible by certain properties of the Falicov-Kimball models (FKM). Upper bounds follow [1] from the Golden-Thompson [5, 6] as well as Hölder [7] inequalities. Upper bounds form a monotonic (non-decreasing)) sequence $\{A_n\}$. The first member thereof ("zeroth" approximant, A_0) needs the knowledge of partition function(s) of the FKM only. It is the simplest one, but also the least precise. The next approximants A_1, A_2... (the first and higher members of the sequence) are more precise, but they need the knowledge of eigenvectors of the FKM.

The lower bounds for the Hubbard model partition function have been obtained with the use of so called Bogoliubov-Peierls inequality [7].

Detailed exposition and proofs can be found in [1], and here we reproduce only formulas for the simplest upper bound as well as for the lower bound:

$$\begin{aligned}\sum_{n} \exp\left(-\beta \sum_{m} \left(E_m^{+} \delta_{mn} + E_m^{-} S_{nm} S_{mn}^{\dagger}\right)\right) \leq \\ \leq Z_{\text{Hub}}(\beta,t,U) \leq Z_{\text{FK}}(2\beta, t, U/2).\end{aligned} \quad (3)$$

where β is the inverse temperature, $E_i^{\pm}$, $v_i^{\pm}$ are energies and eigenvectors of the Falicov-Kimball model with ± particles being mobile, and $S_{ij} = \langle v_i^- | v_j^+ \rangle$. Z_{Hub}, Z_{FK} denote the partition functions of corresponding models with parameters given in parentheses. The sum in l.h.s. of (3) is taken over all eigenstates of the Falicov-Kimball Hamiltonian.

In [1], a preliminary study of precision of these bounds has been undertaken. The calculations were done for $M = 8$ site systems. The full diagonalization was necessary as all energies enter the partition function for non-zero temperature. It has been done by means of the Jacobi method or converting the Hamiltonian matrix to tridiagonal form with subsequent diagonalization [8]. Even for such small systems, the dimension of matrices was up to 4.900 (for half-filled systems). The same technique is used in this paper.

The upper bound $\ln A_0$ for $t = -1$, $\beta = 1$ and various values of U (ranging from $U = 2$ to $U = 1000$) gave an estimation of the free energy for the Hubbard model within 1-20% precision (the logarithms of A_0 and Z_{Hub} have been compared).

The bigger the index n, the better the estimator A_n. For $n = 2^5$, $\ln A_n$ overestimates the $\ln Z_{\mathrm{Hub}}$ by less than one promille.

The lower bound is of less but still reasonable precision within the whole range of the U parameter (usually 10-25%).

III. TEMPERATURE DEPENDENCE OF BOUNDS

We first examine the precision of bounds as a function of temperature. The results are presented in Table 1. It can be seen that the precision of estimators is generally better for higher temperatures (for $\beta = 0.1$, about 1% in all cases, for both lower and upper bounds) and becomes worse in lower temperatures (for $\beta = 10$, up to 40% for upper bound and 70% for lower bound). There are worse cases; in some situations (small and large coupling constants, and for half filling) the precision of estimators is much better even in low temperature region.

Table 1. Some results for 6-site systems with $N_+ = N_- = 3$ obtained by exact diagonalisation of matrices of corresponding Hamiltonians. Periodic boundary conditions have been imposed. $q_n = \ln A_n / \ln Z_{\mathrm{Hub}}$. The behaviour of approximants for low and high temperatures is shown

U	β	q_0	q_1	q_2	q_3	q_4	q_5	L.B.$_{\mathrm{FK}}$	L.B.$_{ff}$
0	0.1	1.0087	1	1	1	1	1	0.99556	1
1	0.1	1.00892	1	1	1	1	1	0.99527	0.99963
2	0.1	1.00913	1	1	1	1	1	0.994476	0.99848
6	0.1	1.0099	1.00005	1.00005	1	1	1	0.992497	0.98497
20	0.1	1.01115	1.00058	1.00016	1.00004	1.00001	1	0.99065	0.78259
100	0.1	1.00359	1.00217	1.00115	1.0004	1.00011	1.00003	0.99638	< 0
1000	0.1	1.00036	1.00035	1.00033	1.0003	1.00025	1.00015	0.99964	< 0
0	1	1.16049	1	1	1	1	1	0.7992	1
1	1	1.185	1.00236	1.00058	1.00015	1.00004	1.00001	0.752178	0.98756
2	1	1.2099	1.01061	1.00274	1.0007	1.00018	1.00004	0.696368	0.942664
6	1	1.25394	1.0900	1.03396	1.00975	1.00253	1.00064	0.68815	0.2493
20	1	1.14459	1.11442	1.08576	1.04498	1.01562	1.00433	0.844007	< 0
100	1	1.03467	1.03326	1.03186	1.02906	1.02352	1.01425	0.96598	< 0
1000	1	1.00359	1.00358	1.00356	1.00353	1.00348	1.00336	0.996403	<< 0
0	10	1.02829	1	1	1	1	1	0.60394	1
1	10	1.05059	1.01351	1.00716	1.00348	1.00142	1.00047	0.44615	0.98019
2	10	1.08789	1.04629	1.02986	1.01598	1.00674	1.00223	0.36742	0.91777
6	10	1.26911	1.24141	1.21608	1.1717	1.10695	1.04608	0.37515	< 0
20	10	1.41014	1.39861	1.38723	1.3649	1.32205	1.24412	0.30041	< 0
100	10	1.25046	1.24993	1.2482	1.24595	1.24147	1.23255	0.7101	<< 0
1000	10	1.03471	1.0347	1.03468	1.03465	1.0346	1.03449	0.96477	<< 0
10000	10	1.00359	1.00359	1.00359	1.00359	1.00359	1.00359	0.99640	<< 0

Table 2. Some results for 8-site systems (lattice 2 × 4) with U negative. $N_+ = N_-$, $\beta = 1$; hopping is allowed only between nearest neighbours; periodic boundary conditions have been imposed

$-U$	N_+	q_0	q_1	q_2	q_3	q_4	q_5	$L.B._{FK}$
2	2	1.13687	1.00557	1.00141	1.00036	1.00009	1.00002	0.81914
6	2	1.07567	1.02491	1.00907	1.00257	1.00067	1.00017	0.904238
10	2	1.03759	1.02139	1.01093	1.00373	1.00103	1.00026	0.956917
20	2	1.01131	1.00892	1.00666	1.00347	1.0012	1.00033	0.98780
100	2	1.0005	1.00048	1.00046	1.00042	1.00034	1.00021	0.99949
2	2	1.1293	1.00577	1.00148	1.00038	1.0001	1.00002	0.82932
6	3	1.06442	1.02173	1.00811	1.00232	1.0006	1.00015	0.9106
10	3	1.03155	1.01823	1.00947	1.00326	1.0009	1.00023	0.96265
20	3	1.00957	1.00756	1.00566	1.00296	1.00103	1.00028	0.98978
100	3	1.00042	1.0004	1.00039	1.00035	1.00029	1.00017	0.99957
2	4	1.13133	1.00545	1.00139	1.00036	1.00009	1.00002	0.841899
6	4	1.05574	1.01842	1.0069	1.00198	1.00051	1.00013	0.92308
10	4	1.026	1.01504	1.00784	1.00271	1.00075	1.00019	0.85879
20	4	1.00778	1.00615	1.00461	1.00241	1.00084	1.00023	0.99183
100	4	1.00035	1.00033	1.00031	1.00028	1.00023	1.00014	0.99966

IV. THE $U < 0$ CASE: MOTIVATION AND RESULTS

The second problem examined in this paper is the behaviour of lower and upper bounds for *negative* values of U. The physical motivation for such a study is the potential applicability of results in the *bosonic* Hubbard model. If the number of both sorts of particles (with up and down spins) is equal, and U is large and negative, one can expect that fermions are completely paired, form bound states and the model is effectively bosonic (with hard-core condition). Therefore, it is interesting to examine the bounds in the case $U < 0$.

The results obtained for 8-site systems and various fillings are presented in Table 2. It turns out that for $|U|$ large, the estimators are *very precise for arbitrary filling even for simplest estimator* A_0. On the ground of existing data one can conjecture that for $|U|$ large, both bounds *saturate*, independently of the filling factor. This is in contrast with the $U > 0$ case, where such a saturation has been observed only at half-filling.

V. SUMMARY AND PERSPECTIVES

In the paper, the numerical study of bounds for the partition function for the Hubbard model has been performed, extending previous calculations. It has been obtained that: *i*) both (upper and lower) bounds are better for high temperatures, and less precise for low temperatures. *ii*) For attracting the Hubbard model ($U < 0$), both bounds are more and more precise with a growing value of $|U|$ (for $|U| = 20$, the precision is about 1%).

As a rule, the observables for the Hubbard model are very hard to calculate. There are only very few rigorous results or reliable numerical methods. For the Falicov-Kimball model, the physical observables are much more calculable (although still not easy to obtain!). For instance, Monte Carlo calculations can always be performed for the Falicov-Kimball model – the fermionic minus-sign problem does not appear here. The upper (A_0 as well as A_1) and lower bounds studied here are actually calculable by the Monte Carlo methods, so the author hopes that they could be useful in studies on the Hubbard model.

The interesting question is an estimation of the *derivatives* of the partition function (magnetization, susceptibilities, specific heat) or, more generally, the *correlation functions*. Estimations obtained in this paper concern only the partition function itself (or equivalently the free energy). Although the partition function is a fundamental object in the statistical mechanics, it is not an object measured immediately in experiments (in contrast with observables like magnetization, etc.). However, it turns out that certain information concerning magnetization *can* be extracted from estimations of partition function! The argument goes as follows:

In the paper [9] it has been shown that if we know the upper bound $f_{UB}(B)$ and the lower bound $f_{LB}(B)$ on the *convex* function $f(B)$, then one can obtain the upper and lower bounds on the derivative $M(B) = \partial f/\partial B$. The free energy for the Hubbard model is a convex function, so we can obtain rigorous upper and lower bounds on magnetization as well as of internal energy. Such estimations have been done in [10] and [11] for the magnetization in the ground state of the HuM. Results of the presented paper could give the estimations of magnetization or internal energy for finite-temperature HuM. The work towards this direction is in progress. One can hope that knowing the partition function with one-percent precision, one could determine the internal energy or magnetization with comparable accuracy. These aspects need further studies.

Some natural areas where estimations obtained in this paper are very accurate and could hopefully be more useful, are:

- Investigation of high-temperature aspects of high-temperature superconductors (fluctuating stripe phases, pseudogap etc.); this region is still poorly understood from theoretically point of view [12];
- Simulations as well as theoretical computations on the area of the *bosonic* Hubbard model.

These aspects will be the subjects of further investigations.

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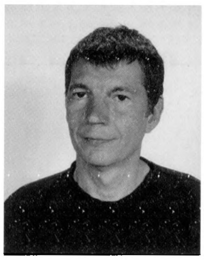

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