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# Estimations of the Free Energy for the Hubbard Model

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**Abstract** A series of upper bounds and two lower bounds for the partition function of the Hubbard model have been derived. These bounds are expressible by certain properties of the Falicov-Kimball model. The upper bounds have been derived mainly by the use of the Golden-Thompson inequality and its generalizations, and the Hölder inequality. The lower bounds are based on the Bogoliubov-Peierls inequality. The numerical values of bounds have also been calculated for small systems.

**Keywords** Hubbard model · Falicov-Kimball model · Lattice fermion systems · Matrix inequalities

## 1 Introduction

The Golden-Thompson inequality [1, 2] turned out to be very useful tool on various areas of statistical mechanics. (Analogous inequality has also been independently proven by Symanzik [3] for the system of anharmonic oscillators). The Golden-Thompson inequality has found numerous applications. Some of them are: convexity of the free energy for general class of quantum statistical models [4], inequalities relating partition functions of various models (for instance, Ising and Heisenberg ones [4]), non-existence of long-range orderings at positive temperatures in $d = 1, 2$ Hubbard models [5].

In this paper, we give some inequalities, estimating the partition function of the Hubbard model (HuM) [6] from above by the properties of the Falicov-Kimball models (FKM) [7] with the use of the Golden-Thompson inequality. These inequalities form a monotonic (non-increasing)) sequence $\{A_n\}$. The first member thereof ("zeroth" approximant, $A_0$) is expressed only by partition function(s) of the FKM only. It is a simplest one, but it is also of least precision. The next approximants $A_1, A_2, \dots$ (the first and higher members of the sequence) are more precise, but they need the knowledge of eigenvectors of the FKM.

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In the paper, the *lower bounds* for the HuM partition function have also been obtained. They have been obtained with the use of so called Bogoliubov-Peierls inequality [4].

Quite a lot of results has been obtained for the upper and lower bound of the HuM ground-state energy; see [8–10] for a representative sample. What concerns the estimation of partition function, the author knows only the reference [11].

The plan of the paper is as follows: Sect. 2 is devoted to upper bounds for the simplest HuM, Sect. 3—to lower ones. In Sect. 4, there are listed more general classes of the Hubbard model, for which bounds derived in Sects. 2 and 3 are still valid. Section 5 contains summary of results and states open problems as well as directions of future investigations. In the Appendix, there are collected matrix inequalities: Golden-Thompson, Hölder, Suzuki-Araki-Hiai and Peierls-Bogoliubov ones, which have been used in the paper.

## 2 Upper Bounds

### 2.1 Simplest Inequalities: Approximant $A_0$

In this Section, we derive inequalities, which estimate the partition function of the HuM from above by the partition function(s) of the FKM. (Equivalently, the free energy of HuM is estimated from below).

#### *2.1.1 Prototype Inequality*

For the sake of simplicity, let us take first the ordinary Hubbard model with n.n. hopping. Its Hamiltonian is:

$$H_{\mathrm{Hub}}(t,U) = -t \sum_{\langle ij\rangle;\sigma=\pm} \left( c^\dagger_{i,\sigma} c_{j,\sigma} + \mathrm{h.c.} \right) + U \sum_i n_{i,+} n_{i,-} \tag{1}$$

where: $i$, $j$ are site indices; we assume that all sites form some finite subset of $\mathbb{Z}^d$. $c^\dagger_{i,\sigma}$ ($c_{i,\sigma}$) are creation (annihilation) operators for fermion with spin $\sigma$ on the $i$-th site; $n_{i,\sigma} = c^\dagger_{i,\sigma} c_{i,\sigma}$ is the particle number operator.

Let us write this Hamiltonian as a sum of two terms:

$$H_{\mathrm{Hub}}(t,U) = H_{\mathrm{FK},+}(t, U-u) + H_{\mathrm{FK},-}(t,u), \tag{2}$$

where

$$H_{\mathrm{FK},+}(t,U) = -t \sum_{\langle ij\rangle} \left( c^\dagger_{i,+} c_{j,+} + \mathrm{h.c.} \right) + U \sum_i n_{i,+} n_{i,-} \tag{3}$$

can be recognized as a Hamiltonian of the *Falicov-Kimball model* with mobile particles "+" and immobile particles "−". Analogously, $H_{\mathrm{FK},-}$ is a Hamiltonian of the FKM with "−" being mobile particles and "+" being immobile ones.

We assume that we are working with $M$-site system, in the sector with fixed number of "plus" and "minus" particles $N_+$, $N_-$. The dimension of the Hilbert space of the system is $\binom{M}{N_+} \cdot \binom{M}{N_-}$.

We have the following chain of (in)equalities:

$$Z_{\mathrm{Hub}}(\beta,t,U) = \mathrm{Tr}\left[ \exp\left(-\beta H_{\mathrm{Hub}}(t,U)\right) \right] \tag{4}$$

$$\le \mathrm{Tr}\left[\exp(-\beta H_{\mathrm{FK},+}(t,U-u))\cdot\exp(-\beta H_{\mathrm{FK},-}(t,u))\right] \tag{5}$$

$$\le \mathrm{Tr}\left[\left|\exp(-\beta H_{\mathrm{FK},+}(t,U-u))\cdot\exp(-\beta H_{\mathrm{FK},-}(t,u))\right|\right] \tag{6}$$

$$\le \sqrt{\mathrm{Tr}\left[\left|\exp(-2\beta H_{\mathrm{FK},+}(t,U-u))\right|\right]\cdot\mathrm{Tr}\left[\left|\exp(-2\beta H_{\mathrm{FK},-}(t,u))\right|\right]} \tag{7}$$

$$= \sqrt{\mathrm{Tr}\left[\exp(-2\beta H_{\mathrm{FK},+}(t,U-u))\right]\cdot\mathrm{Tr}\left[\exp(-2\beta H_{\mathrm{FK},-}(t,u))\right]} \tag{8}$$

$$= \sqrt{Z_{\mathrm{FK},+}(2\beta,t,U-u)\cdot Z_{\mathrm{FK},-}(2\beta,t,u)} \equiv A_0. \tag{9}$$

Some explanations: Passing from (4) to (5) is due to Golden-Thompson inequality; (5) $\Rightarrow$ (6) is due to the fact that $|\mathrm{Tr}(A)| \le \mathrm{Tr}(|A|)$ for arbitrary matrix $A$; (6) $\Rightarrow$ (7) is due to the version (50) of the Hölder inequality; equality of (7) and (8) holds because for arbitrary self-adjoint matrix $H$, the matrix: $\exp(-\beta H)$ is a *positive* one.

This way, we have obtained the prototype inequality:

$$Z_{\mathrm{Hub}}(\beta,t,U) \le \sqrt{Z_{\mathrm{FK},+}(2\beta,t,U-u)\cdot Z_{\mathrm{FK},-}(2\beta,t,u)}. \tag{10}$$

**Particular cases:**

1. When we take $u = U/2$ and $N_+ = N_-$, then $Z_{\mathrm{FK},+}(2\beta,t,U-u) = Z_{\mathrm{FK},-}(2\beta,t,u) \equiv Z_{\mathrm{FK}}(2\beta,t,U/2)$ and the inequality (10) takes the form

$$Z_{\mathrm{Hub}}(\beta,t,U) \le Z_{\mathrm{FK}}(2\beta,t,U/2). \tag{11}$$

   This inequality has been obtained by Brandt [11] from considerations based on convexity properties of the partition function.
2. Putting $u = 0$, we have

$$Z_{\mathrm{Hub}}(\beta,t,U;N_+,N_-) \le \sqrt{Z_{\mathrm{ff}}(2\beta,t;N_-)\cdot Z_{\mathrm{FK},+}(2\beta,t,U;N_+,N_-)} \tag{12}$$

   and analogously, interchanging "plus" and "minus" particles, we obtain a twin inequality

$$Z_{\mathrm{Hub}}(\beta,t,U;N_+,N_-) \le \sqrt{Z_{\mathrm{ff}}(2\beta,t;N_+)\cdot Z_{\mathrm{FK},-}(2\beta,t,U;N_+,N_-)}. \tag{13}$$

   In inequalities above, $Z_{\mathrm{ff}}(2\beta,t;N_\pm)$ denotes the free-fermion partition function for corresponding species of particles; it is given by the lattice Fermi-Dirac distribution.

One can suspect that the inequality (10) is not too optimal. In the Table, a sample of results for small systems is presented. For a wide range of parameters, the value of $\ln(A_0)$ overestimates the $\ln(Z_{\mathrm{Hub}})$ by 10–25%. There is however one important exception: For $U \to \infty$, $\ln(A_0) \to \ln(Z_{\mathrm{Hub}})$ at half filling! So in the limit $U \to \infty$ and for half-filling, the inequality (10) *saturates*. This fact can be explained in a very simple manner. At $U = \infty = u = U - u$ and half-filling (i.e. $N_+ + N_- = M$), both kinds of particles are immobile: hopping becomes completely irrelevant in this case. The partition function of the HuM is equal to $\binom{M}{N_+}$ (the energy of arbitrary state of the system of immobile particles is 0) and for FKM's, $Z_{\mathrm{FK},\pm} = \binom{M}{N_+}$. So, we have an *equality* in the formula (10).

### *2.1.2 Natural Generalization: Inequality Based on General Hölder Inequality*

Passing from (6) to (7), the particular case of the Hölder inequality with $r = 1$, $p = q = 2$ has been used for the sake of simplicity. However, one can use general version (47) of the

Hölder inequality. Then, instead of the inequality (10) one gets

$$\left[Z_{\text{Hub}}(r\beta,t,U)\right]^{\frac{1}{r}} \le \left[Z_{\text{FK},+}(p\beta,t,U-u)\right]^{\frac{1}{p}} \cdot \left[Z_{\text{FK},-}(q\beta,t,u)\right]^{\frac{1}{q}} \tag{14}$$

provided $1 \le p,q,r \le \infty$, and $p^{-1}+q^{-1}=r^{-1}$.

Below we prove inequalities which are better than (10), but they need the knowledge of certain properties of eigenvectors of FK models.

### 2.2 More Refined Inequality: Approximant $A_1$

Let us return to the splitting of the HuM Hamiltonian (2) and the inequality (5) and (6) implied by (2). For the FK Hamiltonian $H_{\text{FK},+}(t,U-u)$ let us denote:

$$|v_i^+\rangle,\, E_i^+ \tag{15}$$

being the $i$-th eigenvector and corresponding $i$-th energy eigenvalue, respectively. Let $\epsilon_i^+ = \exp(-\beta E_i^+)$. Let $|v_i^-\rangle$, $E_i^-$, $\epsilon_i^-$ denote analogous objects for the Hamiltonian $H_{\text{FK},-}(t,u)$.

*Remark*

1. Eigenvectors for FK are easily calculable (one-electron problem in a given external potential).
2. The set of vectors $\{|v_i^+\rangle\}$ form a orthonormal basis. The set: $\{|v_i^-\rangle\}$ also form the orthonormal basis. But basevectors belonging to *different* bases, in general, are *not* orthonormal!

Now let us insert an identity operator written down in two different forms: $I = \sum_i |v_i^+\rangle\langle v_i^+|$, $I = \sum_i |v_i^-\rangle\langle v_i^-|$ into the formula (5). We have:

$$\begin{aligned}
A_1 &\equiv \operatorname{Tr}\left[\exp(-\beta H_{\text{FK},+}(t,U-u)) \cdot \exp(-\beta H_{\text{FK},-}(t,u))\right] \\
&= \sum_{i,j} \langle v_i^-|\exp(-\beta H_{\text{FK},+}(t,U-u))|v_j^+\rangle\langle v_j^+|\exp(-\beta H_{\text{FK},-}(t,u))|v_i^-\rangle \\
&= \sum_{i,j} \langle v_i^-|v_j^+\rangle \epsilon_j^+ \langle v_j^+|v_i^-\rangle \epsilon_i^- \equiv \sum_{i,j} S_{ij}\epsilon_j^+ S_{ji}^\dagger \epsilon_i^- \equiv \operatorname{Tr}(S\mathcal{E}^+ S^\dagger \mathcal{E}^-)
\end{aligned} \tag{16}$$

where $S$ is the matrix of scalar products of elements belonging to the "$-$" and "$+$" bases:

$$S_{ij} = \langle v_i^-|v_j^+\rangle \tag{17}$$

and (no summation over $k$ in the definition of $\mathcal{E}$ below)

$$\mathcal{E}_{jk}^\pm = \epsilon_k^\pm \delta_{kj}. \tag{18}$$

*Remark*

1. The matrix $S$ introduced above is *unitary* because

$$\sum_k S_{ik} S_{kj}^\dagger = \sum_k \langle v_i^-|v_k^+\rangle\langle v_k^+|v_j^-\rangle = \langle v_i^-|v_j^-\rangle = \delta_{ij}.$$

2. One can recognize that during derivation of the equalities (16), the *polar decomposition* of the matrices $\exp(-\beta H_{\mathrm{FK},\pm})$ has been done. More concretely, $\exp(-\beta H_{\mathrm{FK},+}) = S\mathcal{E}^{+}$ and $\exp(-\beta H_{\mathrm{FK},-}) = S^{\dagger}\mathcal{E}^{-}$, where $S$ is unitary and $\mathcal{E}^{+}, \mathcal{E}^{-}$ are positive; in our case they are even diagonal ones.
3. All terms in the sum (16) are *positive*, so one can hope that it would be possible to calculate the approximant $A_1$ by Monte Carlo methods (the partition function of the FKM is calculable by MC; see [15–18]).
4. The expression (16) is nothing else than the certain form of the expression (5), so we have

$$Z_{\mathrm{Hub}}(\beta, t, U) \leq A_1 \leq A_0 \tag{19}$$

   i.e. we have obtained an improvement of the inequality (10).
5. From results in the Table, one can suspect that $A_1 \to Z_{\mathrm{Hub}}$ for $U \to 0$. In fact, it is so, and the proof is very simple: For $U = 0$, the "+" and "−" fermions are *independent* particles, so the matrices $H_{\mathrm{FK},+}$ and $H_{\mathrm{FK},-}$ *commute*. This implies that $\exp(-\beta H_{\mathrm{Hub}}) = \exp(-\beta H_{\mathrm{FK},+})\exp(-\beta H_{\mathrm{FK},-})$, and that inequality: (4)–(5) becomes an equality. Moreover, all eigenvalues and eigenvectors of all matrices involved depend in the continuous matter on parameter(s) ($U$ in our case), which implies that $A_1 \to Z_{\mathrm{Hub}}$ for $U \to 0$.

### 2.3 Further Generalization and Higher Approximants $A_n$

The inequality: $Z_{\mathrm{Hub}}(\beta, t, U) \leq A_1$ obtained in preceding Subsection can be further strengthened. It follows from various generalizations of the Golden-Thompson inequality [12–14]. Using again the division (2) of the Hubbard Hamiltonian into a sum of two FK Hamiltonians and using inequalities (52), we can write

$$\begin{aligned} Z_{\mathrm{Hub}} &= \mathrm{Tr}\left[\exp\left(-\beta H_{\mathrm{Hub}}\right)\right] \\ &\leq \mathrm{Tr}\left[\exp(-\beta H_{\mathrm{FK},+}/p)\cdot\exp(-\beta H_{\mathrm{FK},-}/p)\right]^{p} \equiv A_p = \mathrm{Tr}\left[\left(S\mathcal{E}_p^{+}S^{\dagger}\mathcal{E}_p^{-}\right)^{p}\right] \end{aligned} \tag{20}$$

where

$$(\mathcal{E}_p^{\pm})_{jk} = \exp(-\beta E_k^{\pm}/p)\delta_{kj}, \tag{21}$$

and $S$ is given by (17). Moreover, we have

$$A_0 \geq A_1 \geq A_2 \geq \cdots \geq Z_{\mathrm{Hub}} \tag{22}$$

(the inequality: $A_p \geq A_q$ for $p < q$ follows from the second inequality of (52)).

So, we have obtained a series of upper bounds for the partition function of the HuM. They are expressible by certain objects (traces of products of matrices $S, \mathcal{E}^{\pm}$) related to the FKM's. In the Table there are placed values of the subsequent approximants for small systems. It is however not clear how difficult to calculate are these higher approximants for systems larger than, say, 15 particles ($A_1$ is in principle calculable via Monte-Carlo-like techniques as it is a sum of positive elements. Higher approximants, however are sums of terms with both positive and negative signs).

## 3 Lower Bounds

In preceding sections, we have considered the *upper bounds* for the HuM partition function. It is also possible to obtain the *lower bounds* by the means of so called *Peierls-Bogoliubov* inequality [4].

### 3.1 FK Lower Bound

In the Peierls-Bogoliubov inequality (53), take $A = -\beta H_{\mathrm{Hub}}$. Moreover, let's again use the splitting (2) of the Hubbard Hamiltonian. We have:

$$Z_{\mathrm{Hub}}(\beta, t, U) = \mathrm{Tr}\left(e^{-\beta H_{\mathrm{Hub}}}\right) \geq \sum_n \exp(-\beta\langle\eta_n|H_{\mathrm{Hub}}|\eta_n\rangle)$$
$$= \sum_n \exp(-\beta\langle\eta_n|H_{\mathrm{FK}+} + H_{\mathrm{FK}-}|\eta_n\rangle) \tag{23}$$

where $\{\eta_n\}$ is an arbitrary orthonormal basis. Now, let us choose $\eta_n = v_n^+$, where $v_n^+$ are eigenvectors of the Falicov-Kimball Hamiltonian (see (15)). (The choice $\eta_n = v_n^-$ is another natural one). With this choice, we can write the r.h.s. of (23) as

$$\sum_n \exp(-\beta\langle\eta_n|H_{\mathrm{FK}+} + H_{\mathrm{FK}-}|\eta_n\rangle)$$
$$\equiv LB_{FK} = \sum_n \exp\left[-\beta\left(\langle v_n^+|H_{\mathrm{FK}+}|v_n^+\rangle + \langle v_n^+|H_{\mathrm{FK}-}|v_n^+\rangle\right)\right]$$
$$= \sum_n \exp\left[-\beta E_n^+ - \beta\langle v_n^+|H_{\mathrm{FK}-}|v_n^+\rangle\right]. \tag{24}$$

We can express this quantity in terms of the $S$ matrix (17):

$$\langle v_n^+|H_{\mathrm{FK}-}|v_n^+\rangle = \sum_m \langle v_n^+|v_m^-\rangle\langle v_m^-|H_{\mathrm{FK}-}|v_n^+\rangle = \sum_m E_m^- S_{nm} S_{mn}^\dagger \tag{25}$$

so we can rewrite the r.h.s. of (23) as

$$\sum_n \exp\left(-\beta \sum_m (E_m^+\delta_{mn} + E_m^- S_{nm} S_{mn}^\dagger)\right). \tag{26}$$

In the case $u = U/2$ and $N_+ = N_-$, we have $E_m^+ = E_m^- = E_m$ and rhs takes the form

$$\sum_n \exp\left(-\beta \sum_m E_m(\delta_{mn} + S_{nm} S_{mn}^\dagger)\right). \tag{27}$$

In Table 1, values of this lower bound are given for some baby systems. One can see that in the half-filling case for increasing $U$, the FK-lower bound becomes better, and that the quotient $\ln(Z_{\mathrm{Hub}})/LB_{FK}$ tends to 1 for $U \to \infty$, i.e. the inequality *saturates* in this limit. This fact is again easy to understand: In the case $U = \infty = u = U - u$, both kinds of particles are immobile and all Hamiltonians appearing in (23) (i.e. $H_{\mathrm{Hub}}$, $H_{\mathrm{FK}\pm}$) have common eigenfunctions, being functions of immobile particles. So we have an *equality* in (23).

**Table 1** Some results for 8-site systems for $t = 1$, $\beta = 1$ and with $U$ and filling varied, obtained by numerical diagonalization of matrices of corresponding Hamiltonians. The value of $u$ in the formula (2) has been taken to be $u = U/2$

| $N_+$ | Structure | $U$ | $q_0$ | $q_1$ | $q_2$ | $q_3$ | $q_4$ | $q_5$ | $LB_{FK}$ | $LB_{ff}$ |
|---|---|---|---|---|---|---|---|---|---|---|
| 2 | $2\times 4$, n.n. | 2 | 1.16698 | 1.00396 | 1.00103 | 1.00026 | 1.00007 | 1.00002 | 0.783031 | 0.97414 |
| 2 | $2\times 4$, n.n. | 6 | 1.17287 | 1.01428 | 1.00488 | 1.0014 | 1.00037 | 1.00009 | 0.763377 | 0.829979 |
| 2 | $2\times 4$, n.n. | 20 | 1.17212 | 1.01703 | 1.0086 | 1.00397 | 1.00136 | 1.00038 | 0.823557 | 0.157933 |
| 2 | $2\times 4$, n.n. | 2000 | 1.16807 | 1.00997 | 1.0029 | 1.00085 | 1.00031 | 1.00017 | 0.852819 | $\ll 0$ |
| 2 | $2\times 4$, pyro | 2 | 1.20747 | 1.00375 | 1.00093 | 1.00024 | 1.00006 | 1.00002 | 0.741475 | 0.983815 |
| 2 | $2\times 4$, pyro | 6 | 1.21333 | 1.01628 | 1.00529 | 1.00155 | 1.00041 | 1.0001 | 0.726148 | 0.883773 |
| 2 | $2\times 4$, pyro | 20 | 1.21192 | 1.02589 | 1.01225 | 1.00564 | 1.00195 | 1.00055 | 0.814554 | 0.331745 |
| 2 | $2\times 4$, pyro | 2000 | 1.20405 | 1.01671 | 1.00483 | 1.00143 | 1.00052 | 1.00029 | 0.833634 | $\ll 0$ |
| 3 | $2\times 4$, n.n. | 2 | 1.18245 | 1.00691 | 1.00179 | 1.00046 | 1.00012 | 1.00003 | 0.7517 | 0.9582 |
| 3 | $2\times 4$, n.n. | 6 | 1.19302 | 1.03261 | 1.01169 | 1.00335 | 1.00087 | 1.00022 | 0.723234 | 0.65215 |
| 3 | $2\times 4$, n.n. | 20 | 1.17836 | 1.03638 | 1.02184 | 1.01069 | 1.00367 | 1.00102 | 0.842635 | $< 0$ |
| 3 | $2\times 4$, n.n. | 20000 | 1.158 | 1.01332 | 1.00381 | 1.00102 | 1.00028 | 1.0001 | 0.891526 | $\ll 0$ |
| 3 | $2\times 4$, pyro | 2 | 1.18045 | 1.0066 | 1.00174 | 1.00045 | 1.00012 | 1.00003 | 0.721247 | 0.969418 |
| 3 | $2\times 4$, pyro | 6 | 1.19897 | 1.03575 | 1.01292 | 1.00379 | 1.001 | 1.00025 | 0.67449 | 0.73411 |
| 3 | $2\times 4$, pyro | 20 | 1.18849 | 1.04965 | 1.0298 | 1.01473 | 1.00512 | 1.00142 | 0.820513 | $< 0$ |
| 3 | $2\times 4$, pyro | 2000 | 1.15808 | 1.01789 | 1.00561 | 1.00188 | 1.00089 | 1.00063 | 0.881009 | $\ll 0$ |
| 4 | $2\times 4$, n.n. | 2 | 1.23196 | 1.00962 | 1.00246 | 1.00063 | 1.00016 | 1.00004 | 0.707137 | 0.946119 |
| 4 | $2\times 4$, n.n. | 6 | 1.2513 | 1.08304 | 1.03112 | 1.00892 | 1.00232 | 1.00059 | 0.648649 | 0.282805 |
| 4 | $2\times 4$, n.n. | 20 | 1.13281 | 1.10502 | 1.07867 | 1.04122 | 1.0143 | 1.00396 | 0.8583 | $< 0$ |
| 4 | $2\times 4$, n.n. | 2000 | 1.00161 | 1.00161 | 1.0016 | 1.0016 | 1.00159 | 1.00156 | 0.998387 | $\ll 0$ |
| 4 | $2\times 4$, pyro | 2 | 1.1994 | 1.00902 | 1.00236 | 1.00061 | 1.00016 | 1.00004 | 0.691496 | 0.955858 |
| 4 | $2\times 4$, pyro | 6 | 1.26052 | 1.08723 | 1.0329 | 1.00953 | 1.00249 | 1.00063 | 0.597496 | 0.412359 |
| 4 | $2\times 4$, pyro | 20 | 1.16477 | 1.13041 | 1.09778 | 1.05141 | 1.01789 | 1.00496 | 0.819225 | $<0$ |
| 4 | $2\times 4$, pyro | 2000 | 1.00215 | 1.00214 | 1.00214 | 1.00213 | 1.00211 | 1.00208 | 0.997851 | $\ll 0$ |

Notation: $N_\sigma$—number of particles with spin $\sigma$; we assume $N_+ = N_-$. n.n.— nearest-neighbor hopping; pyro—pyrochlore lattice; $q_n = \ln A_n / \ln Z_{\mathrm{Hub}}$. Periodic boundary conditions have been imposed in every case. The general tendency is that the precision of estimators is better for smaller fillings and smaller coupling constants. For smaller values of the number of sites, the behavior of estimators is similar. For larger temperatures, the precision of estimators is better, and for smaller ones the precision is worse

*Remark* Numerical data suggest that the saturation does *not* hold for fillings other than one-half (see Table 1).

## 3.2 Free Fermion Lower Bound

Another simple lower bound can be obtained with the use of *free fermion* wave functions as an orthonormal system in the Peierls-Bogoliubov inequality. In the Table, values of this lower bound, denoted as $LB_{ff}$ are also given. The inequality *saturates* for $U \to 0$ (notice that for $U \to 0$, the lower bound $LB_{FK}$ does *not* saturate.) The proof is straightforward: For $U = 0$ the free-fermion wave functions are eigenvectors of the $U = 0$ Hubbard Hamiltonian. For $M$ finite, eigenvectors and eigenvalues depend in continuous manner of the parameter(s)

($U$ in our case) and the Peierls-Bogoliubov inequality saturates in the case of the eigenvector basis.

As can be seen from the Table, the free-fermion lower bound is quite accurate for small values of $U$, but becomes useless for moderate and large $U$.

## 4 More General Classes of the Hubbard Model

Inequalities given in preceding Sections are not limited to the standard HuM, given by the formula (1). Below, we list some of other Hamiltonians, for which all inequalities derived above are valid. (An exception is the correlated hopping case, where we have no free-fermion lower bound).

1. *Kinetic term*: One can allow more general form of the kinetic term:

$$T = \sum_{ij;\sigma=\pm} t_{ij} \left( c^{\dagger}_{i,\sigma} c_{j,\sigma} + \text{h.c.} \right). \tag{28}$$

   Notice that translation invariance is not assumed. The dimension and structure of the lattice are also irrelevant.
2. *Potential term*: One can also modify the potential term to more general form, where on-site interaction is site-dependent:

$$V = \sum_i U_i n_{i,+} n_{i,-} \tag{29}$$

3. *Statistics*: All results above are valid for both Fermi and Bose statistics (provided we are working in the framework of the canonical ensemble with finite number of particles).
4. *Chemical potentials*: One can also write analogons of estimations above for the Hubbard model with chemical potentials (i.e. in the grand canonical ensemble). Here matrices of the HuM and FKM are of dimension $4^M$ for one-half spin. For simplicity, let us consider only the standard HuM. Corresponding Hamiltonians are given by

$$H_{\text{Hub}}(t, U, \mu_+, \mu_-) = -t \sum_{\langle ij \rangle;\sigma=\pm} \left( c^{\dagger}_{i,\sigma} c_{j,\sigma} + \text{h.c.} \right) + U \sum_i n_{i,+} n_{i,-} + \mu_+ \sum_i n_{i,+} + \mu_- \sum_i n_{i,-}. \tag{30}$$

   Let us write this Hamiltonian as a sum of two terms:

$$H_{\text{Hub}}(t, U, \mu_+, \mu_-) = H_{\text{FK},+}(t, U-u, \mu_+^{(+)}, \mu_-^{(+)}) + H_{\text{FK},-}(t, u, \mu_+^{(-)}, \mu_-^{(-)}), \tag{31}$$

   where

$$H_{\text{FK},+}(t, U, \mu_+^{(+)}, \mu_-^{(+)}) = -t \sum_{\langle ij \rangle} \left( c^{\dagger}_{i,+} c_{j,+} + \text{h.c.} \right) + U \sum_i n_{i,+} n_{i,-} + \mu_+^{(+)} \sum_i n_{i,+} + \mu_-^{(+)} \sum_i n_{i,-} \tag{32}$$

   and analogously for the $H_{\text{FK},-}(t, U, \mu_+^{(-)}, \mu_-^{(-)})$. Chemical potentials for HuM and FKM's have to satisfy relations : $\mu_+^{(+)} + \mu_+^{(-)} = \mu_+$, $\mu_-^{(+)} + \mu_-^{(-)} = \mu_-$.

For Bose statistics the matter is more delicate (and complicated) as the dimension of the Hilbert space is infinite and one should consider infinite-dimensional analogons of the Golden-Thompson inequality. Author has no statements in this case.

5. *Correlated hopping*: It is possible to include the *correlated hopping* term. In this case, the Hubbard Hamiltonian [6, 19–23], can be split into a sum of two FK Hamiltonians [24–29] in a form analogous as in (2):

$$H_{\mathrm{Hub}}(t,U,a,b)=H_{\mathrm{FK},+}(t,U-u,a,b)+H_{\mathrm{FK},-}(t,u,a,b), \tag{33}$$

$$\begin{aligned} H_{\mathrm{Hub}}(t,U,a,b) = -t \sum_{\langle ij\rangle;\sigma=\pm}\left(c^{\dagger}_{i,\sigma}c_{j,\sigma}+\mathrm{h.c.}\right)\left(1+a(n_{i,-\sigma}+n_{j,-\sigma})+bn_{i,-\sigma}n_{j,-\sigma}\right)\\ +U\sum_i n_{i,+}n_{i,-} \end{aligned} \tag{34}$$

where

$$\begin{aligned} H_{\mathrm{FK},\sigma}(t,U,a,b) = -t \sum_{\langle ij\rangle}\left(c^{\dagger}_{i,\sigma}c_{j,\sigma}+\mathrm{h.c.}\right)\left(1+a(n_{i,-\sigma}+n_{j,-\sigma})+bn_{i,-\sigma}n_{j,-\sigma}\right)\\ +U\sum_i n_{i,+}n_{i,-}. \end{aligned} \tag{35}$$

In formulas above, $a, b$ denote the correlated hopping constants.

6. *Extended Hubbard model*: Consider the Hubbard model with the Hamiltonian, where the Coulomb interaction between particles occupying neighboring sites has been included [6, 30]:

$$H_{\mathrm{Hub}}(t,U,V)=-t\sum_{\langle ij\rangle;\sigma=\pm}\left(c^{\dagger}_{i,\sigma}c_{j,\sigma}+\mathrm{h.c.}\right)+U\sum_i n_{i,+}n_{i,-}+V\sum_{\langle i,j\rangle}n_i n_j \tag{36}$$

(here $n_i = n_{i,+} + n_{i,-}$). This Hamiltonian again can be written as a sum of two (extended) FK models:

$$H_{\mathrm{Hub}}(t,U,V)=H_{FK,+}(t,U/2,V,\alpha)+H_{FK,-}(t,U/2,V,1-\alpha) \tag{37}$$

where $H_{FK,\sigma}$ denotes the Hamiltonian of the FKM with $\sigma$ particles being mobile and $-\sigma$ immobile:

$$\begin{aligned} H_{FK,\sigma}(t,U,V,\alpha) = -t\sum_{\langle ij\rangle}\left(c^{\dagger}_{i,\sigma}c_{j,\sigma}+\mathrm{h.c.}\right)+U\sum_i n_{i,+}n_{i,-}\\ +V\sum_{\langle i,j\rangle}\left[n_{i,-\sigma}n_{j,-\sigma}+\alpha\left(n_{i,\sigma}n_{j,-\sigma}+n_{j,\sigma}n_{i,-\sigma}\right)\right] \end{aligned} \tag{38}$$

$\alpha$ being an arbitrary parameter.

7. *Multiband Hubbard model*: Consider the system in which two species of spin one-half particles (let's call them $d$ and $f$ electrons) are present. Assume that the Hamiltonian describing the system has the following form ("two-band Hubbard model"):

$$H_{\mathrm{Hub};\,df}=T_d+T_f+V_d+V_f+V_{df}+S, \tag{39}$$

where:

$$T_d = -t_d \sum_{\langle ij \rangle;\sigma=\pm} \left( d^\dagger_{i,\sigma} d_{j,\sigma} + \text{h.c.} \right), \qquad T_f = -t_f \sum_{\langle ij \rangle;\sigma=\pm} \left( f^\dagger_{i,\sigma} f_{j,\sigma} + \text{h.c.} \right); \tag{40}$$

$$V_d = U_d \sum_i n_{d;i,+} n_{d;i,-}, \qquad V_f = U_f \sum_i n_{f;i,+} n_{f;i,-}, \qquad V_{df} = U_{df} \sum_i n_{f;i} n_{d;i}; \tag{41}$$

$$S_{\text{Heis}} = -\sum_{i;\alpha} J_\alpha s^\alpha_{f;i} s^\alpha_{d;i}. \tag{42}$$

Here: $\sigma$ is the spin index; $i$ – site index; $n_{a;i} = n_{a;i,+} + n_{a;i,-}$ ($a$ is the band index, so in our case it assumes the values $d$ and $f$); $s^\alpha_{a;i}$ is the *spin operator*, being the bilinear combination of creation and annihilation operators: $s^\alpha_{a;i} = \sum_{\eta,\eta'} \sigma^\alpha_{\eta,\eta'} a^\dagger_\eta a_{\eta'}$, where $\sigma^\alpha_{\eta,\eta'}$ is $\alpha$-th Pauli matrix.

The model defined by (39) and (42) is a slightly generalized two-band Hubbard model with Hund on-site interaction, studied in numerous papers, mainly in the context of metallic ferromagnetism (see [30] for an exhaustive information). Usually one assumes that the Hund interaction is *isotropic*, i.e. all coefficients $J_\alpha$ are equal. A natural generalization is to allow these couplings to be different.

Let us assume now that $J_x = J_y = 0$. With this assumption and moreover $t_f = 0$, the model obtained is called *2-band Hubbard-Ising model* [31, 32]. For this model, there have been obtained rigorous results concerning the existence of ferromagnetism [31] and non-rigorous, but probably exact ones concerning orderings of the ground state [32].

Under assumption: $J_x = J_y = 0$ , we have

$$S_{\text{Is}} = -\sum_i J_z s^z_{f;i} s^z_{d;i} = -\frac{1}{4} \sum_i J_z (n_{f;i,+} - n_{f;i,-})(n_{d;i,+} - n_{d;i,-}) \tag{43}$$

and we can write the Hamiltonian of the Hubbard model as a sum of two Hamiltonians of 2-band Hubbard-Ising models. (In author's opinion, it would be more appropriate to call these models as "the 2-band FK models with anisotropic Hund interactions". But it is not convenient to proliferate new terminology without serious reason, so let's use the existing terminology). So we have

$$H_{\text{Hub};\,df} = H_{\text{HI};d} + H_{\text{HI};\,f}, \tag{44}$$

where

$$H_{\text{HI};d} = T_d + \alpha V_{df} + V_f + \gamma S_{\text{Is}}, \tag{45}$$

$$H_{\text{HI};\,f} = T_f + (1-\alpha) V_{df} + V_d + (1-\gamma) S_{\text{Is}} \tag{46}$$

($\alpha, \gamma$ are arbitrary parameters). $H_{\text{HI};d}$ and $H_{\text{HI};\,f}$ are the Hamiltonians of 2-band Hubbard-Ising models with $d$ and $f$ electrons being mobile, respectively. We again obtain estimations analogous to those proved in preceding sections: (10), (14), (16) and (27).

To complete the picture, it should be mentioned that for numerous interesting models, the author hasn't been able to obtain estimations similar to formulated above (i.e. estimations of HuM partition function by objects related to FKM's). Among these 'harder' model there are: the general multiband Hubbard model and the periodic Anderson model.

## 5 Summary

In the paper, upper and lower bounds for partition functions of the Hubbard model and their extensions have been derived. All of them are rigorous. These bounds are valid for arbitrary parameters such as temperature, filling or coupling constants, and for quite a large class of models. These upper and lower bounds are expressible by certain objects related to corresponding Falicov-Kimball models (partition functions and eigenvectors).

Upper bounds form a whole series $A_n$, which is *monotonic* (non-increasing) and converges to the partition function of HuM for $n \to \infty$. (The convergence follows from the Lie-Trotter formula). The first element of this sequence $A_0$ is the simplest one; it is expressible by partition functions of FKM's. For small systems tested numerically, $\ln A_0$ usually overestimates the $\ln Z_{\text{Hub}}$ by 10–25% for parameters of physical range.

The next upper bound $A_1$ is more precise and usually overestimates the $\ln Z_{\text{Hub}}$ by 1–10%. For the calculation of the $A_1$ it is however needed the knowledge of eigenvectors of the FKM's (more precisely, the scalar products of FKM's with "+" and "−" electrons being mobile). The same quantity is needed to calculate the lower bound. Lower bounds are however of smaller precision: usually, they underestimate the $\ln Z_{\text{Hub}}$ by 10–25%. The fortune opportunity is that both $A_1$ and lower bound can in principle be calculated by Monte Carlo methods.

The bigger the index $n$ the better the estimator $A_n$ is. For $n = 2^5$, $\ln A_n$ overestimates the $\ln Z_{\text{Hub}}$ by less than one promille. However, it is not clear if numerical values of these higher estimators could be determined by some approximate method for M larger than, say, 15 (and comparable number of particles).

There have also been obtained two *lower bounds*, based on the Peierls-Bogoliubov inequality. The first lower bound has been obtained with the use of eigenvectors of the FK models ($LB_{FK}$). It is of reasonable precision within whole range of parameters (usually 10–25%). The second one $LB_{ff}$, based on free-fermion wave functions, is precise for small coupling constant, but useless out of this range.

There have been also observed the *saturation* of certain bounds. For $U \to 0$, both $A_1$ (and of course all higher $A_n$) and $LB_{ff}$ tend to $Z_{\text{Hub}}$. Moreover in the half-filling case for $U \to \infty$, both $A_0$ (and of course all higher $A_n$) and $LB_{FK}$ tend to $Z_{\text{Hub}}$.

The interesting question is an estimation of the *derivatives* of 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.). But it turns out that certain information concerning magnetization *can* be extracted from estimations of partition function! The argument goes as follows:

In the paper [33] 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 easily obtain the upper and lower bounds on the derivative $M(B) = \frac{\partial f}{\partial B}$. The free energy for the Hubbard model is a convex function, so we can obtain rigorous upper and lower bounds on magnetization. Such estimations have been done in [9] and [10] for the magnetization in the ground state of the HuM. Results of the paper presented can give the estimations of magnetization for finite-temperature HuM. The work towards this direction is in progress.

The most interesting problem would be obtaining the *spontaneous* magnetization. The idea is to investigate whether or not a positive lower bound $M_{LB}$: $M(B) \geq M_{LB} > 0$ for $B \to 0$ can be obtained. However, using Fisher construction it is not possible to obtain non-trivial $M_{LB}$ at $B \to 0$, unless curves $f_{UB}(B)$ and $f_{LB}(B)$ coincide. This opportunity suggests that it would be very desirable to improve bounds in such a manner that $f_{UB}(B)$ and $f_{LB}(B)$ coincide.

In the paper, the bounds for the partition function for the Hubbard model have been obtained in terms of the Falicov-Kimball model. In general, there are no explicit expressions for the partition function and other quantities in the FKM (although they can be calculated numerically by the Monte Carlo methods—see [15–18]). In some particular cases, however, the explicit expressions can be obtained. There are: half-filling, $U$ and $\beta$ large (expansions coming from perturbation theory—see [35, 37]); small $U$ expansions [35]; and out of half-filling and $U$ and $\beta$ large, the results in [38, 39] concerning segregation in the FKM. It would be very interesting to use these results in order to obtain explicit bounds for the Hubbard model.

*Concluding remark.* The Hubbard model is a hard one; it is over 40 years old, but both exact results and reliable approximations are still rare. As E. Lieb said, the model is "notoriously difficult" [34]. The Falicov-Kimball model (sometimes called "the simplified Hubbard model") is still difficult, but much more tractable; there exist a number of rigorous results concerning FKM (for a comprehensive reviews, see [35, 36]). Author hopes that upper and lower bounds will be more tractable than the free energy of the Hubbard model, and that inequalities obtained in this paper could give some insight into physics of the Hubbard model.

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## Appendix A: Matrix Inequalities

For proofs and more detailed discussion of matrix inequalities, see excellent publications [4] and [14].

*Hölder inequality for matrices*: If $1 \le p, q, r \le \infty$, and $p^{-1} + q^{-1} = r^{-1}$, then

$$\|AB\|_r \le \left\| A \right\|_p \left\| B \right\|_q \tag{47}$$

where

$$\|A\|_s = \left[\mathrm{Tr}(|A|^s)\right]^{\frac{1}{s}} \tag{48}$$

and

$$|A| = \sqrt{A^\dagger A} \tag{49}$$

is an *absolute value* of the $A$ matrix.

Let us take the inequality (47) for $r = 1$, $p = q = 2$. In this case we have:

$$\|AB\|_1 = \mathrm{Tr}(|AB|) \le \|A\|_2 \|B\|_2 = \sqrt{\mathrm{Tr}(|A|^2) \cdot \mathrm{Tr}(|B|^2)} \tag{50}$$

*The Golden-Thompson inequality*: For $A$, $B$—self-adjoint matrices

$$\mathrm{Tr}\left(e^{A+B}\right) \le \mathrm{Tr}\left(e^A e^B\right). \tag{51}$$

*Generalized Golden-Thompson inequality*: For $A$, $B$—self-adjoint matrices

$$\mathrm{Tr}\left(e^{A+B}\right) \le \mathrm{Tr}\left(e^{A/p} e^{B/p}\right)^p \le \mathrm{Tr}\left(e^{A/q} e^{B/q}\right)^q \quad \text{for } 0 \le q \le p. \tag{52}$$

The first of above inequalities has been proved by Suzuki [12] for $p \in \mathbb{N}$. Both inequalities above (52) follow from more general results due to Araki [13] and Hiai [14]. *Bogoliubov-Peierls inequality* [4]: For $A$—self-adjoint matrix

$$\mathrm{Tr}\left(e^{A}\right) \geq \sum_{n} \exp(\langle \eta_n | A | \eta_n \rangle), \tag{53}$$

where $\{\eta_n\}$ is an arbitrary orthonormal basis.

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