On Lower Bounds for the Free Energy of the Hubbard Model

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Two lower bounds for the free energy of the Hubbard model are compared.

One of the basic tasks in quantum statistics is the calculation the grand thermodynamic potential Ω or Helmholtz free energy F for a given Hamiltonian-operator $\hat{H}$. In almost all cases the free energies cannot be exactly calculated. Thus it is helpful to find upper and lower bounds for the free energies. Upper bounds are mainly based on the inequality [1, 2]

$$\Omega \leq \operatorname{tr} \hat{W}_t(\hat{H}-\mu \hat{N}_e) + \frac{1}{\beta} \operatorname{tr} \hat{W}_t \ln \hat{W}_t , \tag{1}$$

where W_t is a so-called grand canonical trial density matrix, $\hat{N}_e$ is the total number operator and μ is the chemical potential.

In the present note we discuss lower bounds for the Hubbard model. In Wannier representation the Hubbard model is given by

$$\hat{H} = \sum_{ij\sigma} t_{ij} c_{i\sigma}^{\dagger} c_{j\sigma} + U \sum_{i} n_{i\uparrow} n_{i\downarrow} , \tag{2}$$

where the summations are performed over all lattice sites and $n_{i\sigma} = c_{i\sigma}^{\dagger} c_{i\sigma}$ is the number operator. If we assume that the system has cyclic boundary conditions we can express the Hubbard model in Bloch representation, namely

$$\hat{H} = \sum_{\boldsymbol{k}\sigma} \varepsilon_{\boldsymbol{k}} c_{\boldsymbol{k}\sigma}^{\dagger} c_{\boldsymbol{k}\sigma} \tag{3}$$

$$+ \frac{U}{N} \sum_{\boldsymbol{k}_1\boldsymbol{k}_2\boldsymbol{k}_3\boldsymbol{k}_4} \delta(\boldsymbol{k}_1-\boldsymbol{k}_2+\boldsymbol{k}_3-\boldsymbol{k}_4) c_{\boldsymbol{k}_1\uparrow}^{\dagger} c_{\boldsymbol{k}_2\uparrow} c_{\boldsymbol{k}_3\downarrow}^{\dagger} c_{\boldsymbol{k}_4\downarrow} ,$$

where $\boldsymbol{k}$ runs over the first Brillouin zone and δ denotes the Kronecker symbol. The band energy is given by

$$\varepsilon(\boldsymbol{k}) = \sum_{nm} t_{nm} e^{-i(\boldsymbol{R}_n - \boldsymbol{R}_m)} , \tag{4}$$

where t_{nm} is the hopping integral and the $\boldsymbol{R}_n$ are lattice vectors. In the following we assume only hopping to nearest neighbours and consider the half-filled case, i.e. $N_e = N$, where N denotes the number of lattice sites. Only the ground state energy of the Hubbard Hamiltonian operator for the linear chain with cyclic boundary conditions can be found exactly [3] with the help of the Bethe ansatz for $N \to \infty$, $N_e \to \infty$, $n_e = 1$ and $S_z = 0$. For more realistic systems, only approximate solutions can be found for the model.

The grand thermodynamic potential for the Hamiltonian operators

$$\hat{H}_{\text{kin}} = \sum_{\boldsymbol{k}\sigma} \varepsilon_{\boldsymbol{k}} c_{\boldsymbol{k}\sigma}^{\dagger} c_{\boldsymbol{k}\sigma} \tag{5}$$

and

$$\hat{H}_{\text{I}} = U \sum_{i} n_{i\uparrow} n_{i\downarrow} \tag{6}$$

can be calculated exactly [4, 5]. In the first case we find that the grand thermodynamic potential is a lower bound for the grand thermodynamic potential of the Hubbard model, and in the second case we obtain an upper bound for the grand thermodynamic potential of the Hubbard model.

To find further lower bounds we can apply the following theorem [6, 7]:

Theorem: *Let A and B be two $n \times n$ symmetric matrices. Then*

$$\operatorname{tr} e^{A+B} \leq \operatorname{tr} e^{A} e^{B} \leq \tfrac{1}{2} \operatorname{tr} (e^{2A} + e^{2B}) \tag{7}$$

and

$$\operatorname{tr} e^{A+B} \leq \operatorname{tr} e^{A} e^{B} \leq (\operatorname{tr} e^{p_1 A})^{1/p_1} (\operatorname{tr} e^{p_2 B})^{1/p_2} , \tag{8}$$

where $p_1 > 1$ and $p_2 > 1$ with

$$\frac{1}{p_1} + \frac{1}{p_2} = 1 . \tag{9}$$

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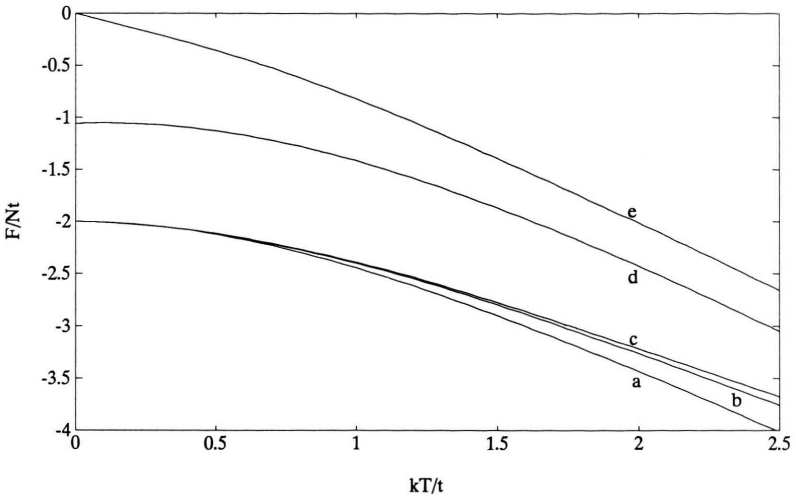

Fig. 1. Helmholtz free energies as functions of temperature with $U/t=4$ for (a) the kinetic part of the Hubbard Hamiltonian, (b) the lower bound derived in this paper for $p_1=p_2=2$, (c) the lower bound derived from the Metha inequality [6], (d) the upper bound derived from the Mermin inequality [2] and (e) the interaction part of the Hubbard Hamiltonian.

The expression on the right hand side of inequality (8) was applied by Steeb [8] to find a lower bound for the grand thermodynamic potential for the half filled case, where the simple cubic lattice has been studied. For a AB lattice the chemical potential μ is given by $\mu=U/2$ in the half filled case. The quantity p_1 was used as a variation parameter. Another option to find a lower bound for the grand thermodynamic potential is to use the expression on the right hand side of inequality (7). A decomposition of the Hamiltonian-operator $\hat{K}=\hat{H}-\mu\hat{N}_e$ to calculate the traces, is

$$A=-\beta(\hat{H}_{\mathrm{kin}}-\tfrac{1}{2}\mu\hat{N}_e),$$
$$B=-\beta(\hat{H}_I-\tfrac{1}{2}\mu\hat{N}_e), \qquad (10)$$

since $A+B=-\beta\hat{K}$. It turns out that this lower bound is worse than the lower bound found from inequality (8). The lower bound can be improved by taking the decomposition

$$A=-\beta(\hat{H}_{\mathrm{kin}}-\lambda\mu\hat{N}_e),$$
$$B=-\beta(\hat{H}_I-(1-\lambda)\mu\hat{N}_e), \qquad (11)$$

where λ is a variational parameter., One has to choose the parameter λ in such a way as to maximize the free energy.

From the theorem given above the question arises whether there is an inequality between the right hand sides of (7) and (8). We prove the following:

Theorem: *Let A and B be two symmetric $n\times n$ matrices. Then*

$$\tfrac{1}{2}\,\mathrm{tr}(e^{2A}+e^{2B})\geq(\mathrm{tr}\,e^{2A})^{1/2}(\mathrm{tr}\,e^{2B})^{1/2}. \qquad (12)$$

Proof: Let $c_1:=\mathrm{tr}\,e^{2A}$ and $c_2:=\mathrm{tr}\,e^{2B}$. Then $c_1>0$ and $c_2>0$. Consequently,

$$\tfrac{1}{4}(c_1-c_2)^2\geq 0. \qquad (13)$$

It follows that

$$\tfrac{1}{4}(c_1^2+c_2^2-2c_1c_2)\geq 0,$$
$$\tfrac{1}{4}(c_1^2+c_2^2+2c_1c_2)\geq c_1c_2,$$
$$\tfrac{1}{4}(c_1+c_2)^2\geq c_1c_2,$$
$$\tfrac{1}{2}(c_1+c_2)\ \geq c_1^{1/2}c_2^{1/2},$$
$$\tfrac{1}{2}\,\mathrm{tr}(e^{2A}+e^{2B})\geq(\mathrm{tr}\,e^{2A})^{1/2}(\mathrm{tr}\,e^{2B})^{1/2}. \qquad (14)$$

In Fig. 1, the Helmholtz free energies for various upper and lower bounds for the Hubbard Hamiltonian are shown for the simple cubic lattice. It reflects the fact that the right hand side of inequality (8) provides one with a better lower bound for the Helmholtz free energy than he right hand side of inequality (7) for $p_1=p_2=2$. It also shows that the lower and upper bounds all improve for higher temperatures. Since the Helmholtz free energy was maximized [8] with respect to p_1 (or p_2) in the calculation of lower bound (8), this lower bound cannot be improved any further.

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