RAPID COMMUNICATIONS

PHYSICAL REVIEW B VOLUME 41, NUMBER 7 1 MARCH 1990

Rigorous bounds on the susceptibilities of the Hubbard model

Kenn Kubo and Tatsuya Kishi
Institute of Physics, University of Tsukuba, Ibaraki 305, Japan
(Received 7 November 1989)

Rigorous bounds on the susceptibilities of the single-band Hubbard model which hold in all dimensions are presented. In the attractive model the spin susceptibility is bounded above by $(4|U|)^{-1}$ where $U(<0)$ is the on-site interaction potential. In the half-filled repulsive model on a bipartite lattice the charge and the on-site pairing susceptibilities are bounded above by U^{-1}. The present result implies that the susceptibilities never diverge in the above-mentioned circumstances and also the absence of corresponding long-range order.

The single-band Hubbard model is an important model in the solid-state theory as the model is thought to involve the essential features of interacting electrons in solids. It is widely believed that the model simulates many interesting phenomena such as ferromagnetism, antiferromagnetism, and metal-insulator transition in appropriate circumstances.[1] Quite recently the possibility of superconductivity in this model has attracted intense interest.[2] In spite of its apparent simplicity and long and intense effort for its understanding, much is left to be clarified except for the one-dimensional case where the exact solution was obtained by Lieb and Wu.[3] According to the exact solution the half-filled repulsive model has a gap in the one-particle excitation spectrum[3] and the charge susceptibility vanishes at zero temperature.[4] In the attractive model electrons form singlet bound states which lead to a gap in the excitation spectrum[3,5] and the vanishing spin susceptibility at $T=0$.[5] In two or three dimensions, on the other hand, the ground state of the half-filled repulsive model is widely believed to have the antiferromagnetic long-range order (AFLRO).[6] The existence of an energy gap is expected in this case as well as in the attractive model. No rigorous result, however, on the existence of AFLRO or energy gap or on the susceptibilities at zero temperature has been known so far.

In this paper we report rigorous upper bounds for some susceptibilities which hold in all dimensions. The first result assures that the spin susceptibility is bounded by $(4|U|)^{-1}$ in the attractive model where $U(<0)$ is the on-site interaction potential. The second result states that the on-site pairing and the charge susceptibilities are bounded by U^{-1} in the half-filled repulsive $(U>0)$ model on a bipartite lattice. As is well known, the Fermi-liquid theory predicts finite spin and charge susceptibilities at $T=0$ where T denotes temperature.[7] On the other hand an exponential decrease of susceptibilities with temperature is expected from the existence of an energy gap. Unfortunately, obtained bounds, which are independent of T, are too loose to say anything on the interesting question whether the model simulates a Fermi liquid or not. Obtained bounds, however, lead to the conclusion that no phase transition leading to corresponding long-range order occurs in above-mentioned circumstances.

Quite recently Lieb proved theorems on the spin state of the ground state of the Hubbard model which hold in all dimensions.[8] According to his result the attractive model with an even number of electrons has a singlet ground state as well as the half-filled repulsive model on a bipartite lattice with the same number of sites in each sublattice. Our result and method are closely related with Lieb, although his argument is confined to the ground state and ours is concerned with finite-temperature properties.

We consider the following Hamiltonian on a finite lattice Λ with $|\Lambda|$ sites

$$H=\sum_{\sigma}\sum_{\alpha\beta\in\Lambda} t_{\alpha\beta}C^{\dagger}_{\alpha\sigma}C_{\beta\sigma}+U\sum_{\alpha\in\Lambda} n_{\alpha\uparrow}n_{\alpha\downarrow}-\sum_{\sigma}\sum_{\alpha\in\Lambda}\mu_{\alpha\sigma}n_{\alpha\sigma}, \tag{1}$$

where $C_{\alpha\sigma}(C^{\dagger}_{\alpha\sigma})$ is the annihilation (creation) operator of an electron with spin σ at the lattice site α and $n_{\alpha\sigma}=C^{\dagger}_{\alpha\sigma}C_{\alpha\sigma}$. The hopping matrix elements $t_{\alpha\beta}$ are assumed to be real and satisfy $t_{\alpha\beta}=t_{\beta\alpha}$. We consider the thermal average over the grand canonical ensemble in the following and the chemical potentials $\mu_{\alpha\sigma}$ are included in H. The spin operators are represented by fermion operators as $S^z_\alpha=(n_{\alpha\uparrow}-n_{\alpha\downarrow})/2$, $S^+_\alpha=C^{\dagger}_{\alpha\uparrow}C_{\alpha\downarrow}$, and $S^-_\alpha=C^{\dagger}_{\alpha\downarrow}\times C_{\alpha\uparrow}$. The density and the on-site pairing operators are given by $n_\alpha=n_{\alpha\uparrow}+n_{\alpha\downarrow}$ and $p_\alpha=C^{\dagger}_{\alpha\uparrow}C^{\dagger}_{\alpha\downarrow}$, respectively. The spin susceptibility with the wave vector $\mathbf{q}$ is given by

$$\chi_{\mathbf{q}}=\beta(S^z_{\mathbf{q}},S^z_{-\mathbf{q}}), \tag{2}$$

with $S^z_{\mathbf{q}}=|\Lambda|^{-1/2}\sum_\alpha S^z_\alpha e^{-i\mathbf{q}\cdot\alpha}$ and (A,B) denotes the Duhamel two-point function

$$(A,B)=\int_0^1 dx\langle e^{\beta xH}Ae^{-\beta Hx}B\rangle .$$

The thermal average is a grand canonical one, i.e., $\langle A\rangle=\Xi^{-1}\mathrm{Tr}(e^{-\beta H}A)$, $\Xi=\mathrm{Tr}(e^{-\beta H})$, where the trace operation is done over the Fock space of electrons on the finite lattice Λ. First we consider the attractive model.

Theorem 1. Assume U is negative and $\mu_{\alpha\sigma}=\mu_\alpha$ (no external magnetic field). No extra assumptions are necessary. Then we can bound the spin susceptibility as

$$\chi_{\mathbf{q}}\leqq(4|U|)^{-1}. \tag{3}$$

Remark 1. Inequality (3) implies the absence of divergence of the spin susceptibility. Using the Falk-Bruch inequality[9] and (3) we obtain an upper bound to the correlation function $\langle S^z_{\mathbf{q}} S^z_{-\mathbf{q}} \rangle$ as

$$\langle S^z_{\mathbf{q}} S^z_{-\mathbf{q}} \rangle \leqq \tfrac{1}{4} C_{\mathbf{q}}^{1/2} |U|^{-1/2} \coth(\beta C_{\mathbf{q}}^{1/2} |U|^{1/2}) , \quad (4)$$

where $C_{\mathbf{q}}$ is any function of $\mathbf{q}$ which has only to satisfy $C_{\mathbf{q}} \geqq \langle (S^z_{\mathbf{q}}, [H, S^z_{-\mathbf{q}}]) \rangle$.[10] If we assume the translational and inversion symmetry of the Hamiltonian, we can adopt, for example, $C_{\mathbf{q}} = (2|\Lambda|)^{-1} \sum_{\mathbf{k}} |2E_{\mathbf{k}} - E_{\mathbf{k}-\mathbf{q}} - E_{\mathbf{k}+\mathbf{q}}|$, where $E_{\mathbf{k}} = \sum_\beta t_{\alpha\beta} e^{i\mathbf{k}\cdot(\alpha-\beta)}$. As a result $\langle S^z_{\mathbf{q}} S^z_{-\mathbf{q}} \rangle$ remains bounded when $|\Lambda| \to \infty$ and therefore there is no magnetic long-range order at any temperature. For the uniform spin correlation function we have $\lim_{\mathbf{q}\to 0} \langle S^z_{\mathbf{q}} S^z_{-\mathbf{q}} \rangle \leqq (4\beta |U|)^{-1}$.

Next we consider the repulsive model on a bipartite lattice.

Theorem 2. Assume U is positive and $\mu_{\alpha\sigma} = U/2$. The lattice Λ is assumed to be bipartite, i.e., $t_{\alpha\beta} \neq 0$ only for pairs of α and β belonging to different sublattices (A and B). Then the charge and the on-site pairing susceptibilities satisfy the following inequalities:

$$\beta(\delta n_{\mathbf{q}}, \delta n_{-\mathbf{q}}) \leqq U^{-1} \quad (5)$$

and

$$\beta(p_{\mathbf{q}}, p_{-\mathbf{q}}) \leqq U^{-1} , \quad (6)$$

where $\delta n_{\mathbf{q}} = n_{\mathbf{q}} - \langle n_{\mathbf{q}} \rangle$ and $n_{\mathbf{q}}(p_{\mathbf{q}})$ is the Fourier transform of $n_\alpha(p_\alpha)$ with wave vector $\mathbf{q}$.

Remarks 2. Under the above assumptions the unitary transformation $C_{\alpha\sigma}(C^\dagger_{\alpha\sigma}) \to \eta_\alpha C^\dagger_{\alpha\sigma}(\eta_\alpha C_{\alpha\sigma})$, where $\eta_\alpha = 1$ for $\alpha \in A$ and -1 for $\alpha \in B$, does not change the Hamiltonian.[3] As $n_{\alpha\sigma}$ is transformed to $1 - n_{\alpha\sigma}$, $\langle n_{\alpha\sigma} \rangle = \frac{1}{2}$ is deduced, i.e., the system is half-filled.

Remarks 3. According to (5) and (6) the charge and the on-site pairing susceptibility do not diverge at a finite temperature. Also by using the Falk-Bruch inequality we can prove the absence of corresponding long-range order at any temperature. We conclude, therefore, no phase transition leading to charge-density wave or on-site Cooper pairing occurs in the half-filled repulsive model on a bipartite lattice.

Proof of Theorem 1. Proof follows straightforwardly that of the Gaussian domination in the quantum spin systems.[10] Define for a set of real numbers $\{h_\alpha\}$,

$$\Xi(\{h_\alpha\}) = \mathrm{Tr}\left[\exp\left(K_\uparrow + K_\downarrow - \tfrac{1}{2}\beta|U| \sum_{\alpha\in\Lambda} (n_{\alpha\uparrow} - n_{\alpha\downarrow} - h_\alpha)^2\right)\right] , \quad (7)$$

where

$$K_\sigma = -\beta \sum_{\alpha\beta\in\Lambda} t_{\alpha\beta} C^\dagger_{\alpha\sigma} C_{\beta\sigma} + \beta \sum_{\alpha\in\Lambda} [\mu_{\alpha\sigma} - (U/2)] n_{\alpha\sigma} .$$

We leave $\mu_{\alpha\sigma}$ dependent on σ. Using the Trotter formula we rewrite as $\Xi(\{h_\alpha\}) = \lim_{n\to\infty} \alpha_n$, where

$$\alpha_n = \mathrm{Tr}\left\{\left[\exp(K_\uparrow/n)\exp(K_\downarrow/n) \prod_{\alpha\in\Lambda} \exp\left(-\frac{\beta U}{2n} \sum_{\alpha\in\Lambda} (n_{\alpha\uparrow} - n_{\alpha\downarrow} - h_\alpha)^2\right)\right]^n\right\} .$$

The operator identity $\exp(-A^2) = (4\pi)^{-1/2} \int \exp(ikA)\exp(-k^2/4) dk$ leads to

$$\alpha_n = (4\pi)^{-n|\Lambda|/2} \int d^{n|\Lambda|}k \exp\left(-\sum_{i=1}^{n} \sum_\alpha (k^2_{\alpha,i}/4 + i\epsilon_n k_{\alpha,i} h_\alpha)\right) \beta_{n\uparrow} \beta^*_{n\downarrow} , \quad (8)$$

where $\beta_{n\sigma}$ is the trace of a product of $n(|\Lambda|+1)$ operators as

$$\beta_{n\sigma} = \mathrm{Tr}_\sigma \left[\prod_{i=1}^{n} \left(\exp(K_\sigma/n) \prod_\alpha \exp(i\epsilon_n k_{\alpha,i} n_{\alpha\sigma})\right)\right] ,$$

$\epsilon_n = (\beta|U|/2n)^{1/2}$ and Tr_σ denotes the trace operation over the Fock space of σ-spin electrons on the lattice Λ. Here we have made use of the fact that K_σ and $n_{\alpha\sigma}$ operate as the identity operator in the Fock space of $-\sigma$-spin electrons and are represented by real matrices since $t_{\alpha\beta}$ is real. Applying Schwarz inequality to (8) and the operator identity in the reversed way and noting the Fock spaces for up and down spins are identical, we have $|\alpha_n|^2 \leqq \delta_{n\uparrow}\delta_{n\downarrow}$, where

$$\delta_{n\sigma} = \mathrm{Tr}\left\{\left[\exp(K_\sigma/n)\exp(K'_{-\sigma}/n) \prod_{\alpha\in\Lambda} \exp\left(-\frac{\beta U}{2n} \sum_{\alpha\in\Lambda} (n_{\alpha\uparrow} - n_{\alpha\downarrow})^2\right)\right]^n\right\}$$

and K'_σ is given by replacing $\mu_{\alpha\sigma}$ with $\mu_{\alpha-\sigma}$ in K_σ as

$$K'_\sigma = -\beta \sum_{\alpha\beta\in\Lambda} t_{\alpha\beta} C^\dagger_{\alpha\sigma} C_{\beta\sigma} + \beta \sum_{\alpha\in\Lambda} [\mu_{\alpha-\sigma} - (U/2)] n_{\alpha\sigma} .$$

Taking the limit $n \to \infty$ we obtain

$$\Xi(\{h_\alpha\})^2 \leqq \Xi_\uparrow \Xi_\downarrow , \quad (9)$$

where

$$\Xi_\sigma = \mathrm{Tr}\left[\exp\left(K_\sigma + K'_{-\sigma} - \tfrac{1}{2}\beta|U| \sum_{\alpha\in\Lambda} (n_{\alpha\uparrow} - n_{\alpha\downarrow})^2\right)\right] .$$

For $\mu_{\alpha\uparrow} = \mu_{\alpha\downarrow} = \mu$, we have $\Xi(\{h_\alpha\}) \leqq \Xi$ for any real $\{h_\alpha\}$. Expanding $\Xi(\{h_\alpha\})$ up to second order in $\{h_\alpha\}$ and extending the result to complex $\{h_\alpha\}$ using the relation (A,B)

$=(B,A)$, we have

$$\left(\sum_\alpha h_\alpha S^z_\alpha, \sum_\alpha h^*_\alpha S^z_\alpha\right) \leqq (4\beta|U|)^{-1}\sum_\alpha |h_\alpha|^2 . \quad (10)$$

If we choose $h_\alpha = |\Lambda|^{-1/2} e^{-i\mathbf{q}\cdot\alpha}$ we obtain inequality (3), QED.

Proof of Theorem 2. We make use of a unitary transformation which transforms the repulsive model to an attractive one, i.e., $C_{\alpha\downarrow}(C^\dagger_{\alpha\downarrow}) \rightarrow \eta_\alpha C^\dagger_{\alpha\downarrow}(\eta_\alpha C_{\alpha\downarrow})$, while the spin-up operators are not altered.[3,8] Then the Hamiltonian (1) is transformed to $\tilde{H}$ where

$$\tilde{H} = \sum_\sigma \sum_{\alpha\beta\in\Lambda} t_{\alpha\beta} C^\dagger_{\alpha\sigma} C_{\beta\sigma} - U \sum_{\alpha\in\Lambda} n_{\alpha\uparrow} n_{\alpha\downarrow} - \sum_{\alpha\in\Lambda} [(\mu_{\alpha\uparrow} - U) n_{\alpha\uparrow} - \mu_{\alpha\downarrow} n_{\alpha\downarrow}] - \sum_{\alpha\in\Lambda} \mu_{\alpha\downarrow} .$$

If $U>0$ and $\mu_{\alpha\uparrow} = \mu_{\alpha\downarrow} = U/2$, $\tilde{H}$ is the attractive model with the chemical potential $-U/2$, for which Theorem 1 holds. As n_α is transformed to $1+2S^z_\alpha$ the charge susceptibility $\beta(\delta n_\mathbf{q}, \delta n_{-\mathbf{q}})$ is transformed to $4\beta(S^z_\mathbf{q}, S^z_{-\mathbf{q}})$ of $\tilde{H}$ and we obtain inequality (5). On the other hand, the pairing operator p_α is transformed to $\eta_\alpha S^+_\alpha$. The rotational invariance of $\tilde{H}$ in the spin space and Theorem 1 immediately leads to inequality (6), QED.

Remarks 4. It is obvious that the proofs for Theorems 1 and 2 can be generalized to the cases where the on-site interaction potential U varies with site on the lattice. In those cases inequality (10) is modified and we cannot necessarily express the result in a compact form with a single wave vector **q**.

Remarks 5. Putting $h_\alpha \equiv 0$ and $\mu_{\alpha\sigma} = \mu + \epsilon_\sigma B$ [$\epsilon_\sigma = 1(-1)$ for $\sigma = \uparrow(\downarrow)$] in inequality (9) we can immediately prove $\langle(\sum_\alpha S^z_\alpha)^2\rangle \leqq \langle(\sum_\alpha \delta n_\alpha)^2\rangle/4$ for $U<0$, i.e., the spin fluctuation is suppressed compared to the charge fluctuation in the attractive model. Also the one-site relation $(S^z_\alpha, S^z_\alpha) \leqq (\delta n_\alpha, \delta n_\alpha)/4$ holds for $U<0$. Inequalities in the opposite direction hold in the half-filled repulsive model on a bipartite lattice.

We thank S. Takada for helpful advice and encouragement. We are indebted to T. A. Kaplan and M. Takahashi for useful discussions.

---

[1]See, for example, papers in *Electron Correlation and Magnetism in Narrow-Band Systems,* edited by T. Moriya (Springer-Verlag, Berlin, 1981), and references therein.

[2]For example, C. Gros, R. Joynt, and T. M. Rice, Z. Phys. B **68**, 425 (1987); H. Q. Lin, J. E. Hirsch, and D. J. Scalapino, Phys. Rev. B **37**, 7359 (1988); H. Shimahara and S. Takada, J. Phys. Soc. Jpn. **57**, 1044 (1987); M. Imada, *ibid.* **56**, 3793 (1987); **57**, 3128 (1988); S. R. White, D. J. Scalapino, R. L. Sugar, N. E. Bickeres, and R. T. Scalettar, Phys. Rev. B **39**, 839 (1989).

[3]E. H. Lieb and F. Y. Wu, Phys. Rev. Lett. **20**, 1445 (1968).

[4]T. Usuki, N. Kawakami, and A. Okiji, Phys. Lett. A **135**, 476 (1989); N. Kawakami, T. Usuki, and A. Okiji, *ibid.* **137**, 287 (1989).

[5]M. Takahashi, Prog. Theor. Phys. **42**, 1098 (1969); **43**, 1619 (1970); **44**, 348 (1970); **45**, 756 (1971); **52**, 103 (1974).

[6]K. Kubo and M. Uchinami, Prog. Theor. Phys. **54**, 1289 (1975); J. E. Hirsch, Phys. Rev. B **31**, 4403 (1985).

[7]L. D. Landau, Zh. Eksp. Teor. Fiz. **30**, 1058 (1957) [Sov. Phys. JETP **3**, 920 (1957)].

[8]E. H. Lieb, Phys. Rev. Lett. **62**, 1201 (1989).

[9]H. Falk and L. W. Bruch, Phys. Rev. **180**, 442 (1969).

[10]F. J. Dyson, E. H. Lieb, and B. Simon, J. Stat. Phys. **18**, 335 (1978).