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LETTER TO THE EDITOR

Thermodynamics of the strongly correlated Hubbard model

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Abstract. High-temperature expansions for the specific heat and susceptibility of the *strongly correlated Hubbard model* are compared with corresponding quantities for spinless free fermions and free spins. It is found numerically that, when the temperature is high, the ratio of the specific heat of the strongly correlated Hubbard model to that of spinless free fermions approaches a particle-density-dependent constant. For fixed temperature, the susceptibility of the Hubbard model is less (greater) than that of free spins when the particle density is below (above) a certain threshold density of approximately 0.7. The ratio of the susceptibilities for the two systems, however, appears to be finite for any value of the particle density. Given that the free spin system does not have a ferromagnetic state at any finite temperature, it is concluded that the strongly correlated Hubbard model does not have a finite phase transition temperature. This conclusion is consistent with our recent high-temperature expansion studies.

The single-band strongly correlated Hubbard model [1] is theoretically important as it is one of the simplest non-trivial models of interacting fermions. There is, however, no common agreement as to whether the model has a phase transition. Some authors believe that below a certain critical hole density, the model has a ferromagnetic or anti-ferromagnetic ground state for dimensionality $d > 2$ [2–4]. On the other hand, from high-temperature expansions, it is found that the model does not have a ferromagnetic state at any finite temperature on hypercubic lattices [5, 6]. Recently, Yedidia [7] compared high-temperature expansions of the strongly correlated Hubbard model with those of spinless free fermions and free spins on two- and three-dimensional lattices. In this paper, we present further comparisons of the strongly correlated Hubbard model with spinless free fermions and free spins on both finite- and infinite-dimensional lattices.

The single-band strongly correlated Hubbard model is described by the Hamiltonian [8]

$$\mathscr{H}^{(H)} = -t \sum_{\langle ij\rangle} \sum_{\sigma=\uparrow,\downarrow} (\tilde{a}^{\dagger}_{i\sigma}\tilde{a}_{j\sigma} + \tilde{a}^{\dagger}_{j\sigma}\tilde{a}_{i\sigma}) - h \sum_{i=1}^{N} (n_{i\uparrow} - n_{i\downarrow}) \tag{1}$$

where $\langle ij\rangle$ denotes nearest-neighbour lattice sites, $\tilde{a}_{i\sigma} = a_{i\sigma}(1 - n_{i-\sigma})$ and $\tilde{a}^{\dagger}_{i\sigma} = (1 - n_{i-\sigma})a^{\dagger}_{i-\sigma}$. $a^{\dagger}_{i\sigma}$ and $a_{i\sigma}$ are Fermi creation and annihilation operators at site i with spin σ. The first term in (1) is the kinetic energy with a nearest-neighbour hopping energy t and zero otherwise. The second term represents the interaction between the electron's spin with an external field h. The factor $1 - n_{i-\sigma}$ associated with $a^{\dagger}_{i\sigma}$ and $a_{i\sigma}$ prevents double occupancy of lattice sites.

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The spinless free fermion Hamiltonian is given by

$$\mathscr{H}^{(0)} = -t \sum_{\langle ij \rangle} (a_i^\dagger a_j + a_j^\dagger a_i) \tag{2}$$

where $a_i^\dagger$ and a_i are fermion creation and annihilation operators at site i.

The kinetic energies in (1) and (2) are similar insofar as double occupancy of a site is excluded, with particles otherwise free to move to neighbouring sites. The specific heat, which measures temperature variation of the internal energy, should thus be similar for the two systems. The difference comes from the existence of spin correlations in the Hubbard model. That is, particles hopping along the same lattice trajectories in both models have different Boltzmann weights. However, when the particle density is low, the probability that two particles meet each other is small and hence correlation effects should be small. We found in fact that, when the temperature T is high, the ratio of the specific heat for the strongly correlated Hubbard model to that of spinless free fermions approaches a constant which depends only on the particle density and approaches unity in zero particle density limit.

The grand canonical partition function for spinless free fermions is

$$Z_G^{(0)} = \mathrm{Tr}\, \mathrm{e}^{-\beta\mathscr{H}^{(0)} + \beta\mathscr{N}} \tag{3}$$

where $\mathscr{N} = \Sigma\, n_i$ is the total particle number operator. Defining

$$z \equiv \mathrm{e}^{\beta\mu} \qquad p \equiv \frac{z}{1+z} \tag{4}$$

we find, after Fourier transformation, that the Gibbs free energy per site is given by

$$g^{(0)} = -\frac{1}{N\beta} \ln Z_G^{(0)} = \frac{1}{\beta}\ln(1-p) - \frac{1}{N\beta}\sum_k \ln[1 + p(\mathrm{e}^{-\beta\varepsilon_k} - 1)] \tag{5}$$

where

$$\varepsilon_k = -2t \sum_{i=1}^{d} \cos k_i. \tag{6}$$

The expansion coefficients $a_m^{(2n)}$ for the Gibbs free energy are defined by

$$g^{(0)} = \frac{1}{\beta}\ln(1-p) - \frac{1}{\beta}p(1-p) \sum_{n=1}^{\infty} \frac{\tau^{2n}}{(2n)!} \sum_{m=0}^{2n-2} a_m^{(2n)} p^m. \tag{7}$$

After some manipulation, we have

$$a_m^{(2n)} = \begin{cases} 0 & \text{when } m<0 \text{ or } m>2n-2 \\ a_{m-1}^{(2n)} + \dfrac{(-1)^m}{m+1} S_{n,m+1} K_{2n} & \text{when } 0 \leqslant m \leqslant 2n-2 \end{cases} \tag{8}$$

where $S_{n,m}$ is given by

$$S_{n,1} = 1 \qquad S_{n,m} = m^n - \sum_{l=1}^{m-1} \frac{m!}{(m-l)!\,l!} S_{n,m-l} \quad \text{when } 2 \leqslant m \leqslant n \tag{9}$$

and K_{2n} is given by

$$K_{2n} = \sum_{n_1+n_2+\ldots+n_d=n} \frac{2^{2n}(2n)!}{(2n_1)!(2n_2)!\ldots(2n_d)!} I_{2n_1} I_{2n_2} \ldots I_{2n_d} \qquad I_{2m} = \frac{(2m)!}{2^{2m} m!^2}. \tag{10}$$

In the infinite-dimensional limit, on the other hand, the hopping integral t is replaced by $td^{-1/2}$ and the expansion coefficients for the Gibbs free energy $a_m^{(2n)}$ are given in the limit by

$$a_m^{(2n)} = \begin{cases} 0 & \text{when } m<0 \text{ or } m>2n-2 \\ a_{m-1}^{(2n)} + \dfrac{(-1)^m}{m+1}\dfrac{(2n)!}{n!} S_{n,m+1} & \text{when } 0 \leqslant m \leqslant 2n-2. \end{cases} \tag{11}$$

Using standard thermodynamic relations [9], the particle density $\rho^{(0)}$ and the specific heat $C_V^{(0)}$ for spinless free fermions can be derived from a knowledge of the Gibbs free energy. Thus if we write

$$\rho^{(0)} = p + p(1-p) \sum_{n=1}^{\infty} \frac{\tau^{2n}}{(2n)!} \sum_{m=0}^{2n-1} D_m^{(2n)} p^m \tag{12}$$

and

$$C_V^{(0)} = kp(1-p) \sum_{n=1}^{\infty} \frac{\tau^{2n}}{(2n)!} \sum_{m=0}^{2n-2} c_m^{(2n)} p^m = k\rho^{(0)}[1-\rho^{(0)}] \sum_{n=1}^{\infty} \frac{\tau^{2n}}{(2n)!} \sum_{m=0}^{2n-2} C_m^{(2n)} [\rho^{(0)}]^m \tag{13}$$

where k is the Boltzmann constant, p can be eliminated between (7) and (12) and the Gibbs free energy can also be expanded in particle density as

$$g^{(0)} = \frac{1}{\beta} \ln(1-p) - \frac{1}{\beta} \rho^{(0)}[1-\rho^{(0)}] \sum_{n=1}^{\infty} \frac{\tau^{2n}}{(2n)!} \sum_{m=0}^{2n-2} A_m^{(2n)} [\rho^{(0)}]^m. \tag{14}$$

The expansion coefficients in (14) for the square lattice and infinite-dimensional hypercubic lattice are tabulated in tables 1 and 2 respectively.

To compare the specific heats for the two systems, we choose units in which $t=1$ and $k=1$, and plot the ratios of the specific heats as functions of the temperature for different particle densities as shown in figure 1. It is apparent from the figure that, when the temperature is high, the ratio approaches a constant which depends only on the particle density.

The magnetic properties of the strongly correlated Hubbard model, on the other hand, are similar to those of free localized spins. The difference again comes from spin correlations in the Hubbard model which arise from hopping. The total magnetic moment, however, is only dependent on the number of up and down spins. In fact, the susceptibility of free spins is simply $\beta\rho$ which is the lowest-order term in the susceptibility expansion for the Hubbard model.

The actual values of the susceptibilities for the two systems, however, are close, as is seen from figure 2, with the difference diminishing rapidly as the temperature increases. Figure 2 also reveals that the difference is smaller for higher orders of expansions. This suggests that the ratio of the susceptibilities for the two systems is finite for any particle density ρ. Padé analysis [10] of $\chi^{(H)}/\chi^{(F)}$ as a function of T for $0.05 \leqslant \rho \leqslant 0.95$ indicates no sign of a physical singularity in the positive T axis. As the free spin system does not have a ferromagnetically ordered phase at any finite temperature in any dimensions, we conclude that the strongly correlated Hubbard model does not have a ferromagnetic phase transition temtemperature in any dimensions. This conclusion is consistent with our earlier high-temperature expansion studies [5, 6].

Following the method by Yedidia, and using the known data for the high-temperature expansions of the strongly correlated Hubbard model [5, 11], we calculated the particle densities where the specific heat (magnetic susceptibility) expansion

Table 1. High-temperature expansion coefficients of spinless free fermions on the square lattice.

	$2n$	$i=0$	$i=1$	$i=2$	$i=3$	$i=4$	$i=5$	$i=6$	$i=7$	$i=8$	$i=9$
$a_i^{(2n)}$	2	4									
	4	36	-216	216							
	6	400	-12000	60000	-96000	48000					
	8	4900	-617400	8849400	-41160000	82320000	-74088000	24696000			
	10	63504	-32387040	1152597600	-11842225920	52969956480	-120982740480	147867793920	-92177326080	23044331520	
$c_i^{(2n)}$	2	8									
	4	48	-1056	1056							
	6	480	-37440	371520	-668160	334080					
	8	5600	-1888320	42262080	-287024640	659205120	-618831360	206277120			
	10	70560	-76305600	5056228800	-70870464000	401898067200	-1039477017600	1346028364800	-856745164800	214186291200	
$D_i^{(2n)}$	2	4	-8								
	4	36	-504	1296	-864						
	6	400	-24800	216000	-624000	720000	-288000				
	8	4900	-1244600	28400400	-200037600	617400000	-938448000	691488000	-197568000		
	10	63504	-64901088	3554953920	-51979294080	324060912000	-1043716181760	1881953740800	-1920360960000	1036994918400	-230443315200
$A_i^{(2n)}$	2	4									
	4	-60	168	-168							
	6	1840	-6240	8160	-3840	1920					
	8	-94780	157640	924280	-4280640	7432320	-6350400	2116800			
	10	7371504	23052960	-366458400	1390798080	-2635355520	2831915520	-1783918080	719953920	-179988480	
$C_i^{(2n)}$	2	8									
	4	-144	-288	288							
	6	4800	43200	-100800	115200	-57600					
	8	-258720	-6099520	14002240	-7902720	-15805440	23708160	-7902720			
	10	20684160	1007899200	-1098619200	-7003584000	27212371200	-44547148800	41673139200	-22992076800	5748019200	

Table 2. High-temperature expansion coefficients of spinless free fermions on the infinite-dimensional hypercubic lattice.

	$2n$	$i=0$	$i=1$	$i=2$	$i=3$	$i=4$	$i=5$	$i=6$	$i=7$	$i=8$	$i=9$
$a_i^{(2n)}$	2	2									
	4	12	-72	72							
	6	120	-3600	18000	-28800	14400					
	8	1680	-211680	3034080	-14112000	28224000	-25401600	8467200			
	10	30240	-15422400	548856000	-5639155200	25223788800	-57610828800	70413235200	-43893964800	10973491200	
$c_i^{(2n)}$	2	4									
	4	48	-480	480							
	6	720	-44640	269280	-449280	224640					
	8	13440	-4273920	79107840	-407070720	847042560	-772208640	257402880			
	10	302400	-463881600	22403606400	-262623513600	1253322201600	-2956833331200	3669645772800	-2300601139200	575150284800	
$D_i^{(2n)}$	2	2	-4								
	4	12	-168	432	-288						
	6	120	-7440	64800	-187200	216000	-86400				
	8	1680	-426720	9737280	-68584320	211680000	-321753600	237081600	-67737600		
	10	30240	-30905280	1692835200	-24752044800	154314720000	-497007705600	896168448000	-914457600000	493807104000	-109734912000
$A_i^{(2n)}$	2	2									
	4	-12	24	-24							
	6	120	0	0	0	0					
	8	-1680	23520	-265440	725760	-967680	725760	-241920			
	10	30240	0	-43545600	377395200	-1146700800	1799884800	-1683763200	928972800	-232243200	
$C_i^{(2n)}$	2	4									
	4	0	-288	288							
	6	0	-14400	129600	-230400	115200					
	8	0	-752640	27847680	-176117760	392878080	-365783040	121927680			
	10	0	-43545600	5617382400	-92142489600	507741696000	-1279718092800	1636095283200	-1036733644800	259183411200	

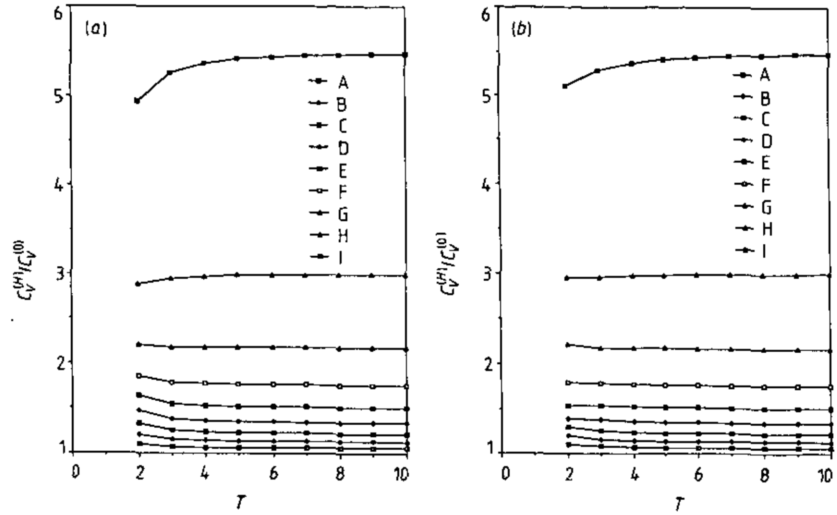

Figure 1. Ratio of the specific heat of the strongly correlated Hubbard model to that of spinless free fermions for different particle densities as a function of the temperature. The specific heat is expanded to order of τ^8 on the square lattice and to order of τ^{10} on the infinite-dimensional hypercubic lattice. A–I correspond to particle densities $\rho = 0.1$–0.9. (*a*) Square lattice. (*b*) Infinite-dimensional hypercubic lattice.

coefficient of τ^{2n} for spinless free fermions (free spin system) is equal to that of the Hubbard model. The results for $2 \leqslant 2n \leqslant 8$ on the square lattice and for $2 \leqslant 2n \leqslant 10$ on infinite-dimensional hypercubic lattice are listed in table 3 and are consistent with the above discussions.

In summary, high-temperature expansions for the strongly correlated Hubbard model have been compared numerically with those of spinless free fermions and those of the free spin system. When the temperature is high, the ratio of the specific heat of

Table 3. The particle densities ρ_{C_V} where the coefficients of τ^{2n} of $C_V^{(H)} - C_V^{(0)}$ is equal to zero and ρ_χ where the coefficients of τ^{2n} of $\chi^{(H)} - \chi^{(F)}$ is equal to zero.

d	$2n$	ρ_{C_V}	ρ_χ
2	2	any	any
	4	0.727 27	0.727 27
	6	0.759 60	0.768 00
	8	0.791 93	0.803 52
3	2	any	any
	4	0.727 27	0.727 27
	6	0.729 45	0.745 66
	8	0.733 92	0.762 81
∞	2	any	any
	4	0.727 27	0.727 27
	6	0.703 86	0.728 32
	8	0.678 18	0.721 27
	10	0.652 90	0.715 14

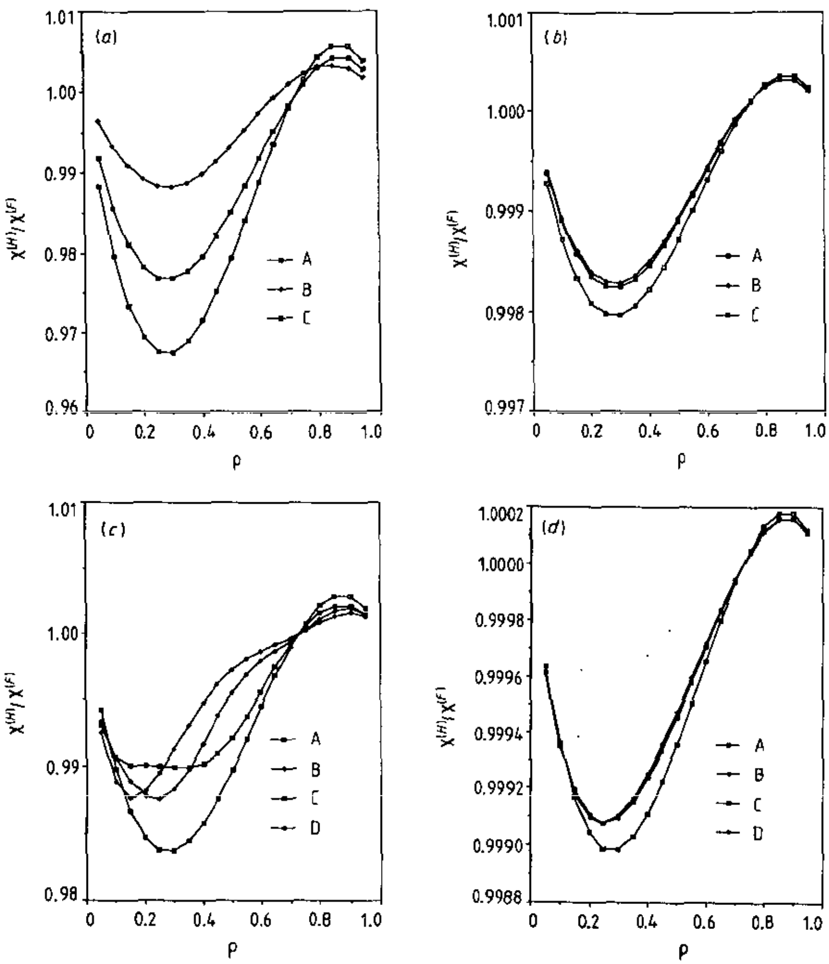

Figure 2. Ratio of the zero-field magnetic susceptibility of the strongly correlated Hubbard model to that of free spin system for different temperatures as a function of the particle density. The susceptibilities for the strongly correlated Hubbard model are expanded to order of τ^8 on the square lattice and to order of τ^{10} on the infinite dimensional hypercubic lattice. A–I correspond to particle densities $\rho = 0.1$–0.9. (*a*) and (*b*) correspond to $T = 1.5$ and $T = 3$ on square lattice. (*c*) and (*d*) correspond to $T = 1.5$ and $T = 3$ on the infinite-dimensional hypercubic lattice.

the strongly correlated Hubbard model to that of spinless free spins approaches a particle-density-dependent constant. On the other hand, the ratio of the susceptibility of the strongly correlated Hubbard model to that of free spin system is finite for any particle density. From the fact that the free spin system does not have a ferromagnetically ordered phase at any finite temperature, we conclude that the strongly correlated Hubbard model does not have a finite ferromagnetic phase transition temperature in any dimensions. This conclusion is consistent with our earlier high-temperature expansion studies.

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