The effects of quantum fluctuations in the large-U Hubbard model at half-filling

1994 J. Phys.: Condens. Matter 6 L53

(http://iopscience.iop.org/0953-8984/6/6/004)

J. Phys.: Condens. Matter 6 (1994) L53–L58. Printed in the UK

LETTER TO THE EDITOR

The effects of quantum fluctuations in the large-U Hubbard model at half-filling

M Di Stasio†, E Ercolessi‡, G Morandi§ and A Tagliacozzo†¶

† SISSA–ISAS via Beirut 2, I-34100 Miramare, Trieste, Italy

‡ Physics Department, Syracuse University, Syracuse, NY 13244-1130, USA

§ Dipartimento di Fisica, Universita' di Bologna, INFM and INFN via Irnerio 46, 1-40126 Bologna, Italy

¶ Dipartimento di Scienze Fisiche, Universita' di Napoli INFM, Mostra d'Oltremare Padiglione 19, I-80125 Napoli, Italy

Received 8 November 1993

Abstract. A quantitative estimate of the role of quantum fluctuations is given at zero and finite temperatures within the one-loop approximation around the antiferromagnetic and dimer saddle points. Our results include the constraint of single occupancy of sites, also for thermodynamical quantities.

The limit of the large-U Hubbard model at half filling is the spin-$\frac{1}{2}$ antiferromagnetic (AFM) Heisenberg model. In this work we report results of thermal and quantum fluctuations on an AFM background, and in dimer-ordered phases starting from a fermionic representation of the Hamiltonian [1]. Here the constraint of a single-site occupancy is a crucial ingredient.

While quantum Monte Carlo approaches are restricted to relatively small systems [2], analytical methods to include the constraint originate from the Gutzwiller projection [3].

The constraint is often implemented within the saddle-point approximation by a Lagrange multiplier (or slave bosons away from half filling [4]). However it is hard to control its fluctuations both at zero and at finite temperatures. We have implemented it, at all temperatures, with a new method [5], by means of a local chemical potential.

The fluctuations are calculated within the one-loop approximation around the chosen saddle point for an effective action.

We find that, in the AFM case, because the magnetization acts as a local mean field, our method guarantees that the constraint is fully satisfied at the mean-field level. In fact the mean square fluctuations of the occupancy $(n_i^2 - 1)$ vanish at all temperatures when the constraint is evaluated by the saddle-point approximation. At zero temperature, the results of spin-wave theory for the AFM ground state energy are recovered.

Zero-point fluctuations in the staggered and columnar dimer phases were first discussed by Read and Sachdev [6] within the SU(N) model. We show that their results in the $N = 2$ limit do not differ from a fermionized theory in the absence of the constraint. In this case the fluctuations are unrealistically large. This is because unconstrained fermionization of spin operators enlarges the Hilbert space enormously in the case of the dimer phases, due to the opportunity given to the bond field to build up couplings to states which change the site occupancy. This implies that the mean-field free energy of the dimer phases is lowered too much, unless the constraint is enforced.

0953-8984/94/060053+06$07.50

We show that application of the constraint raises the mean-field energy and reduces the fluctuations. However our approximations in dealing with it depress the mean average thermal fluctuations of the occupancy number in the dimer phase up to only 10% of the unconstrained value [7]. Evidently this is not enough because the energies we obtain are still too low compared with what is expected [8].

On the other hand while the saddle-point effective action cannot be promoted to a free energy when the constraint is added, we show that by including fluctuations, a physically meaningful temperature dependence is recovered. Figure 2 reports our results for the specific heat versus temperature.

At half filling the spin-$\frac{1}{2}$ AFM Heisenberg Hamiltonian can be rewritten, in the restricted Hilbert space with single-site occupancy, as

$$H_0 = -\frac{J}{2}\sum_{(i,j)}\sum_{\alpha\beta} c^{\dagger}_{i,\alpha}c_{j,\alpha}c^{\dagger}_{j,\beta}c_{i,\beta} - \frac{NJ}{2} \tag{1}$$

where the sum is over ordered nearest neighbour (NN) pairs of sites in the lattice and N is the number of sites.

The partition function within the subspace of singly occupied states is

$$\mathcal{Z} = \mathrm{Tr}\left\{\prod_i n_i(2-n_i)\mathrm{e}^{-\beta H_0}\right\} \tag{2}$$

where $n_i = n_{i\uparrow} + n_{i\downarrow}$; $n_{i\sigma} = c^{\dagger}_{i\sigma}c_{i\sigma}$, $\sigma = \uparrow, \downarrow$. To implement the constraint we add a source term [5] to the Hamiltonian H_0 and define: $H[z_i] = H_0 - \beta^{-1}\sum_i z_i n_i$ (the z_i are real variables). We call $\mathcal{Z}[z_i]$ the generating functional of averages of the occupation numbers. The partition function of (2) can be recovered as

$$\mathcal{Z} = \prod_i \frac{\partial}{\partial z_i}(2 - \frac{\partial}{\partial z_i})\mathcal{Z}[z_i]\Big|_{z=0}. \tag{3}$$

The advantage is that the evaluation of $\mathcal{Z}[z_i]$ only requires standard techniques because the trace is unrestricted and the source term commutes with H_0. The last feature is lost away from half filling.

The Hubbard Stratonovich decoupling of H_0 requires an auxiliary field in imaginary time (denoted generically by $\mathbf{U}$ in the following), depending on the saddle point chosen:

$$\sum_{\beta} c^{\dagger}_{j,\beta}c_{i,\beta} \to \mathcal{U}_{ij}(\tau) \qquad \text{(flux and dimer phases)}$$

$$c^{\dagger}_{i,\alpha}c_{i,\beta} \to \sum_q \gamma_q^{1/2}\mathrm{e}^{\mathrm{i}qR_i}\mathbf{M}_q(\tau)\cdot\sigma_{\alpha\beta} \qquad \text{(AFM phase)}. \tag{4}$$

Here $\mathcal{U}^*_{ij}(\tau) = \mathcal{U}_{ji}(\tau)$, the components of σ are the Pauli matrices and $\gamma_q = \sum_{\mathrm{NN}}\mathrm{e}^{\mathrm{i}qR} = \cos q_x + \cos q_y$.

The π–flux phase [9] has been discussed by us elsewhere [7]. We have found that temperature destabilizes it more easily than the dimer phases due to the lower-lying excitations. However this phase, together with an AFM background was found to be a good starting point for Monte Carlo calculations at low doping [10]. the order parameter $\mathcal{U}_{ij}$ of the staggered and columnar dimer phases are sketched in figure 1. Integrating out the fermions, one arrives at the intermediate result

$$\mathcal{Z}[z_i] = \int \prod_{(i,j)} \mathcal{D}\mathcal{U}_{ij} \exp\left(-\pi\sum_{(ij)}\sum_m |\mathcal{U}_{i,j}(\Omega_m)|^2 + \mathrm{Tr}\ln[1 + G_0\mathbf{U}]\right). \tag{5}$$

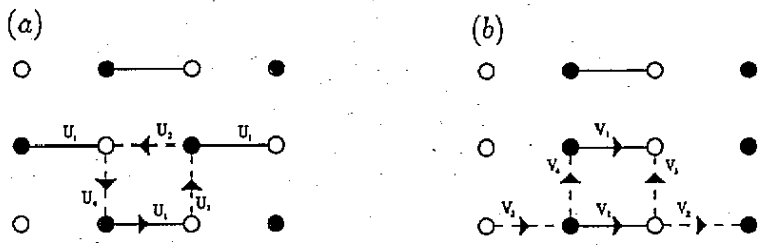

Figure 1. Pictorial representation of the link order parameter U in terms of (*a*) U_1, U_2, U_3, U_4 for the staggered dimer phase (periodicity is along the diagonals), and (*b*) V_1, V_2, V_3, V_4 for the columnar dimer phase (periodicity is doubled on the x axes). Reversing the arrows implies complex conjugation.

Where $\Omega_m = \omega_{n'} - \omega_n$ is a Bose-like Matsubara frequency,

$$(\mathbf{U}^{\mathrm{AF}})_{ij}^{\alpha\beta}(\Omega_m) = \delta_{i,j}\left(z_i\delta_{m,0}\delta_{\alpha\beta} - 2\sum_q e^{iqR_i}\left(\frac{-\pi\beta J\gamma_q}{N}\right)^{1/2}\mathbf{M}_q(\Omega_m)\cdot\sigma_{\alpha\beta}\right) \tag{6}$$

for the AFM phase, while:

$$(\mathbf{U}^{d})_{ij}^{\alpha\beta}(\Omega_m) = \delta_{\alpha,\beta}\left(z_i\delta_{m,0}\delta_{i,j} - \left(\frac{\pi\beta J}{2}\right)^{1/2}\mathcal{U}_{i,j}(\Omega_m)\right) \tag{7}$$

for the dimer phases. Also, G_0 is the Green function in the absence of $\mathcal{U}$ ($(G_0)_{ij}^{nn'} = (i\omega_n)^{-1}\delta_{i,j}\delta_{n,n'}$). Inserting this result into (3), we eventually obtain:

$$\mathcal{Z} = \int\prod_{(i,j)}\mathcal{D}\mathcal{U}_{ij}\exp\left(-\pi\sum_{(i,j)}\sum_m|\mathcal{U}_{ij}(\Omega_m)|^2 + \mathrm{Tr}\ln[1+G_0\mathbf{U}] + \sum_i\ln 4B_i[\mathbf{U}]\right)_{z_i=0}. \tag{8}$$

The contribution of the constraint is represented by the last term of (8) with

$$B_i[\mathbf{U}] = \mathrm{Tr}\{[\chi G_0 P_i]^2\} + 2\,\mathrm{Tr}\{\chi G_0 P_i\} - (\mathrm{Tr}\{\chi G_0 P_i\})^2. \tag{9}$$

Here $\chi = (1+G_0\mathbf{U})^{-1}|_{z_i=0}$ and we have introduced the projector P_i onto the ith site of the lattice, whose matrix elements are $(P_i)_{jk} = \delta_{jk}\delta_{ij}$.

We now expand the action to second order around the mean-field saddle point: $\mathcal{F} = \mathcal{F}^0 + \mathcal{F}^{(2)}$. The second variation $\mathcal{F}^{(2)}$ is given by:

$$\beta\mathcal{F}^{(2)} = \pi\int_0^1 d\tau\ \mathrm{Tr}\{(\delta\mathcal{U})^2\} - \frac{1}{2}\mathrm{Tr}(\chi\delta\mathcal{U}\chi\delta\mathcal{U}) - \frac{1}{2}\sum_i\left(\frac{\delta^2 B_i}{B_i} - \frac{(\delta B_i)^2}{B_i^2}\right). \tag{10}$$

The eigenvalues $\lambda(m)$ of the quadratic form are listed in table 1, for the case without the constraint, together with their degeneracy and the component admixture which is present in the eigenvector. They are functions of Ω_m and are expressed in terms of the mean-field order parameters M (magnetization) and d (dimer bond). The functions $E(m)$, $F(m)$ also appear, defined as

$$F(m) = \frac{2M|\gamma_q|}{\sqrt{\Omega_m^2 t^2 + (4M)^2}} \qquad E(m) = \frac{4d^2}{\Omega_m^2 t^2 + 4d^2} \tag{11}$$

where $t = 1/\beta J$. In the case of the AFM phase, the longitudinal mode decouples with respect to the transverse ones. The collective excitation spectrum can be obtained from the latter. In fact, one has to continue analytically the product $\lambda_+^{\mathrm{AF}}\cdot\lambda_-^{\mathrm{AF}}$ for $i\Omega_m \to \beta\omega + i0$ and look for the zeros. The spin-waves dispersion is recovered in this way, that is: $\omega_q = 2MJ\sqrt{(1-(\gamma_q/2)^2)}$.

In the case of the dimer phase, the second variation $\mathcal{F}^{(2)}$ can be expressed in terms of the complex variations $u_l(Q)$ $(l = 1, 4)$ for the staggered and $v_l(Q)$ for the columnar phase which are the Fourier transforms of $\mathcal{U}(i, \tau)$ and are taken to depend on site and time (with $Q \equiv (\mathbf{Q}, \Omega_m)$). Here i spans just one of the sublattices, according to figure 1. In this case there is no $\mathbf{Q}$ dependence of the eigenmodes.

In table 1 the zero modes are also indicated in the absence of the constraint. However, the features that we will discuss in the following are preserved by the inclusion of the constraint. The AFM phase has a vanishing eigenvalue for $\mathbf{q} = 0$ and $\mathbf{q} = (\pi, \pi) = \pi$ due to the self-consistent equation for the magnetization M. For the dimer phases there is one zero mode which corresponds to an overall change of the phase of the component of the order parameter $d = \langle \mathcal{U}_1 \rangle$. In addition to this, the second variation of the action around the columnar phase saddle point is found to be flat versus two more amplitude deviations which add a small opposite weight on vertical bonds (mixing of the real or imaginary parts of v_3 and v_4), leading to a ladder pattern for the order parameter. Quartic terms in the deviations, that are neglected here, would guarantee that the columnar-phase minimum is stable.

The free energy per particle of the AFM phase, in units of J, is

$$f^{\mathrm{AF}} = f_0^{\mathrm{AF}} + \frac{2t}{N} \sum_q^{\mathrm{RBZ}} \sum_{m \geqslant 0} \ln \lambda_+^{\mathrm{AF}}(m) \lambda_-^{\mathrm{AF}}(m) + \frac{t}{N} \sum_q^{\mathrm{RBZ}} \sum_{m \geqslant 0} \ln \lambda_l^{\mathrm{AF}}(m). \tag{12}$$

The zero-temperature limit is the well-known result of the first $(1/S)$ correction

$$f_{(t=0)}^{\mathrm{AF}} = f_0^{\mathrm{AF}} + \frac{2}{N} \sum_q^{\mathrm{RBZ}} \left(\sqrt{(1 - (\gamma_q/2)^2)} - 1 \right) \tag{13}$$

where $f_0^{\mathrm{AF}} = 2(M^2 - M) = -0.5$, $(M = \frac{1}{2})$ and the correction due to the fluctuations is -0.158. Addition of the constraint does not change the zero-temperature results but it does change the thermodynamical quantities (see figure 2).

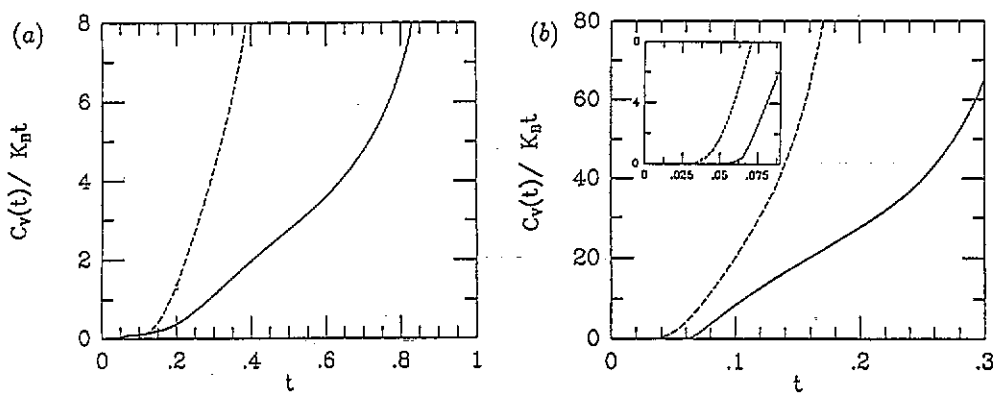

Figure 2. Temperature dependence of the specific heat $c(T)$ for the AFM phase (a) and the staggered dimer phase (b). Full curves include the constraint while the broken ones do not.

In the case of the staggered dimer phase, the closed form for the free energy is

$$f^s = f^0 - \frac{t}{2} \ln C^s + \frac{t}{4} \sum_{m>0} \ln \lambda_1^s(m) + \frac{3t}{2} \sum_{m \geqslant 0} \ln \lambda_2^s(m) + \frac{t}{4} \sum_{m \geqslant 0} \ln \lambda_3^s(m) \tag{14}$$

where the constant $C^s = 2d(2\pi/t)^{1/2}$ arises from the zero-mode integration.

Table 1. Eigenvalues of the second variation of the effective action, as functions of the Matsubara frequencies Ω_m, for the dimer and antiferromagnetic phases together with their degeneracy and the corresponding admixture of the fluctuating fields. The constraint is not included. Modes that vanish for $\Omega = 0$ are explicitly indicated. All the quantities are defined in the text.

	$\lambda\ (\ m \neq 0)$	$\lambda(m=0)$		deg.	mixture
ANTIFERROMAGNETIC PHASE	$\lambda_+^{AF} = 1 - F(m)$	$1 - \dfrac{\gamma(\vec{q})\tanh M\ t}{4M}$ 'zero modes $\vec{q}$=0,$\vec{\pi}$'		2	$m_x(\vec{q}), m_y^x(\vec{q}+\vec{\pi})$
	$\lambda_l^{AF} = 1$	$1 + \dfrac{\gamma(\vec{q})}{2t\cosh^2 M/t}$		2	$m_z(\vec{q})$
	$\lambda_-^{AF} = 1 + F(m)$	$1 + \dfrac{\gamma(\vec{q})\tanh M/t}{4M}$		2	$m_x^x(\vec{q}+\vec{\pi}), m_y(\vec{q})$
STAGGERED DIMERS	$\lambda_1^S = 1 - E(m)$	$1 - \dfrac{1}{2d}\tanh\dfrac{d}{2t} = 0$ 'zero mode'		1	$u_1(\vec{Q}), u_1(-\vec{Q})$
	$\lambda_2^S = 1 - \dfrac{E(m)}{2}$	$1 - \dfrac{1}{2}\left(\dfrac{1}{2d}\tanh\dfrac{d}{2t} + \dfrac{1}{4t\cosh^2 d/2t}\right)$		6	$u_i(\vec{Q})$ i = 2,3,4
	$\lambda_3^S = 1$	$1 - \dfrac{1}{4t\cosh^2 d/2t}$		1	$u_1(\vec{Q}), u_1(-\vec{Q})$
COLUMNAR DIMERS	$\lambda_1^C = 1 - E(m)$	$1 - \dfrac{1}{2d}\tanh\dfrac{d}{2t} = 0$	'zero mode'	1	$v_1(\vec{Q}), v_1(-\vec{Q})$
			'flat second variation'	2	v_3^R, v_4^R v_3^I, v_4^I
	$\lambda_2^C = 1 - \dfrac{E(m)}{2}$	$1 - \dfrac{1}{2}\left(\dfrac{1}{2d}\tanh\dfrac{d}{2t} + \dfrac{1}{4t\cosh^2 d/2t}\right)$		2	$v_2(\vec{Q})$
	$\lambda_3^C = 1$	$1 - \dfrac{1}{4t\cosh^2 d/2t}$		3	$v_1(\vec{Q}), v_1(-\vec{Q})$ v_3^R, v_4^R v_3^I, v_4^I

For the columnar phase we get:

$$f^c = f^0 - \frac{t}{2}\ln C^c + \frac{3t}{4}\sum_{m>0}\ln\lambda_1^c(m) + \frac{t}{2}\sum_{m\geqslant 0}\ln\lambda_2^c(m) + \frac{3t}{4}\sum_{m\geqslant 0}\ln\lambda_3^c(m) \tag{15}$$

where $C^c = 2^3 d(2\pi/t)^{3/2}$. The saddle-point free energy f^0 is equal for the two phases. Its zero-temperature value is: $f^0 = d^2 - d - 1/2 = -3/4$ $(d = 0.5)$ without the constraint. Imposing the constraint this value rises to $f^0 = -0.375$, that is the energy per particle of a collection of spin singlets.

The contribution of quantum fluctuations to the free energy at zero temperature, in the absence of the constraint, is

$$\Delta f^{s}_{(t=0)} = -\frac{d}{4} - 6\left(\frac{d}{4}\right)(1 - 1/\sqrt{2}) \qquad \text{(staggered)}$$
$$\Delta f^{c}_{(t=0)} = -3\left(\frac{d}{4}\right) - 2\left(\frac{d}{4}\right)(1 - 1/\sqrt{2}) \qquad \text{(columnar)}. \tag{16}$$

The factors 6, 3 and 2 come from the degeneracies of the eigenvalues. This result, derived first by Read and Sachdev [6] within the $1/N$ expansion, implies that the degeneracy of the staggered and the columnar phases is broken by quantum fluctuations and that the last one is favoured energetically.

The eigenvalues mostly contributing to lower the energy for both periodicities are $\lambda_1^{s,c}(m \neq 0)$. The presence of two extra amplitude modes of this kind in the columnar phase implies that the energy is lower in this case.

We only report here the analytical zero-temperature result with the constraint included

$$\Delta f^{s}_{(t=0)} = -2d(1 - 1/\sqrt{2}) \qquad \text{(staggered)}$$
$$\Delta f^{c}_{(t=0)} = -\frac{d}{2} - d(1 - 1/\sqrt{2}) \qquad \text{(columnar)}. \tag{17}$$

In the $t = 0$ limit the constraint only affects the contribution of the zero-mode eigenvalues and partially lifts the degeneracy of $\lambda_1^c(m)$. Summing up, the constraint raises the zero-temperature energies including one-loop corrections from the values of -1.095 (staggered phase) and -1.198 (columnar phase) up to -0.668 and -0.771 respectively. Although these values become comparable with the AFM result, within the same approximations, they are still lower than the AFM one, which is commonly accepted to be wrong [8]. We believe that fluctuations can be further depressed when the constraint is dealt with at a higher level of approximation.

At finite temperatures, we have calculated the constraint violation within mean field, which is found to be about 10%. Its action is evident in the temperature dependence of the specific heat, as can be seen from figure 2(a, b). Spin waves dominate the specific heat of the AFM phase, which therefore remains quadratic in temperature close to $t = 0$, while the gapped spectrum of the dimer phase gives an exponential temperature dependence as seen in the inset of figure 2(b). The zero modes, being dispersionless in the dimer phases, do not change the gapped nature of the excitation spectrum. The figures show that our method of including the constraint up to one-loop corrections gives consistent finite-temperature results.

References

[1] Arovas D P and Auerbach A 1988 *Phys. Rev.* B **38** 316
[2] Loh E Y and Gubernatis J E 1990 *Electron Phase Transitions* ed W Hanke and Y V Kopaeve (New York: North-Holland)
[3] Gros C 1989 *Ann. Phys., NY* **189** 53
[4] Kotliar G and Ruckenstein A E 1986 *Phys. Rev. Lett.* **57** 1362
[5] Di Stasio M, Ercolessi E, Morandi G, Tagliacozzo A and Ventriglia F 1992 *Phys. Rev.* B **45** 1939
[6] Read N and Sachdev S 1989 *Nucl. Phys.* B **316** 609
[7] Di Stasio M, Ercolessi E, Morandi G, Tagliacozzo A and Ventriglia F 1993 *Int. J. Mod. Phys.* B **7** 3281
[8] Manousakis E 1991 *Rev. Mod. Phys.* **63** 1
[9] Affleck I and Marston J B 1988 *Phys. Rev.* B **37** 3774
Affleck I 1989 *Phys. Rev.* B **39** 11538
[10] Hsu T C 1990 *Phys. Rev.* B **41** 11379