Magnetic and pairing correlations in correlated electron systems

1996 J. Phys.: Condens. Matter 8 5691

(http://iopscience.iop.org/0953-8984/8/31/002)

J. Phys.: Condens. Matter **8** (1996) 5691–5702. Printed in the UK

Magnetic and pairing correlations in correlated electron systems

Gang Su†

Institut für Theoretische Physik, Universität zu Köln, Zülpicher Strasse 77, D-50937 Köln, Germany

Received 6 February 1996, in final form 25 March 1996

Abstract. Magnetic and superconducting pairing correlation functions in a general class of Hubbard models, the t–J model and a single-band Hubbard model with additional bond–charge interaction are investigated. Some rigorous upper bounds of the corresponding correlation functions are obtained. It is found that the decay of the spin–spin correlation function with temperature in the general Hubbard models cannot be slower than the inverse square law at low temperatures and the inverse law at high temperatures, while the on-site pairing correlation function cannot be slower than the inverse law. An upper bound for the average energy of the t–J model is found. The upper bounds for the spin–spin and the electron pairing correlation functions in the t–J model as well as in the Hubbard model with bond–charge interaction are also obtained. These bounds are expected to provide certain standards for approximate methods. In some special cases, these bounds rule out the possibility of corresponding magnetic and pairing long-range order.

1. Introduction

The study of superconductivity and magnetism in strongly correlated electron systems has been receiving intense interest recently. This may be attributed to the discovery of high-temperature superconductivity. Since the idea of explaining superconductivity in the framework of strongly correlated electron systems (the Hubbard model and its variants) was proposed [1], numerous investigations of these systems have been made. For the many-body problems, which are difficult to solve, only a few rigorous results are known in the literature [2]. Most researchers used approximate or numerical methods to investigate spin and pairing correlation functions, and usually achieved different—sometimes even conflicting—results. In addition, some difficulties in the numerical methods remain unsolved. Therefore, the answers to a variety of interesting questions regarding these systems remain ambiguous to date. In this situation, it is really necessary to search for some exact results which, on the one hand, can be used to examine the validity of some kinds of approximation or numerical calculation, and on the other hand, can help us to further understand the physical properties of these systems.

In this paper, we will study magnetic and pairing correlation functions in the following systems: a general class of Hubbard models, the t–J model and a single-band Hubbard model with additional bond–charge interaction. By using Bogoliubov's inequality, we give some upper bounds for the correlation functions studied, which, to some extent, may provide

† On leave from: Graduate School, Chinese Academy of Sciences, Beijing, People's Republic of China.

0953-8984/96/315691+12$19.50

certain checks and standards for approximate methods. In some special cases, these bounds rule out the possibility of the corresponding magnetic long-range order (LRO) and the on-site pairing LRO.

The rest of the paper is organized as follows. In section 2 a general class of Hubbard models are studied. Symmetries of correlation functions are discussed. The upper bounds for the magnetic correlation function and the on-site pairing correlation function are presented. In sections 3 and 4, the magnetic and pairing correlation functions in the t–J model and a single-band Hubbard model with bond–charge interaction are discussed. A simple upper bound for the average energy of the t–J model is obtained. The upper bounds for the spin–spin correlation functions and the pairing correlation functions in the two models are given. In section 5 a summary of the results is presented.

2. Hubbard models

Consider a general class of Hubbard models on a d-dimensional lattice with M (even) sites. The Hamiltonian is

$$H = \sum_{r,r'} t_{r,r'}(a_r^\dagger a_{r'} + b_r^\dagger b_{r'}) + \sum_r U_r a_r^\dagger a_r b_r^\dagger b_r - \sum_r \mu_r (a_r^\dagger a_r + b_r^\dagger b_r) \qquad (2.1)$$

where $t_{r,r'}$ is the hopping matrix element, and satisfies $t^*_{r,r'} = t_{r',r}$. a_r (b_r) annihilates a spin-up (spin-down) electron at site r, U_r is the local spin-independent Coulomb potential, and μ_r is the position-dependent chemical potential. No other *a priori* assumption (apart from those indicated explicitly in the context) is needed. This is thus a very general form of the Hubbard model.

Define the local spin operators as follows: $S_r^+ = a_r^\dagger b_r$, $S_r^- = b_r^\dagger a_r$, $S_r^z = \frac{1}{2}(n_r^a - n_r^b)$ with $n_r^a = a_r^\dagger a_r$ and $n_r^b = b_r^\dagger b_r$, and $[S_r^+, S_{r'}^-] = 2S_r^z \delta_{r,r'}$, $[S_r^\pm, S_{r'}^z] = \mp S_r^\pm \delta_{r,r'}$. The global spin operators $S^\pm = \sum_r S_r^\pm$ and $S^z = \sum_r S_r^z$ obey the usual SU(2) symmetry and satisfy $[S^\pm, H] = [S^z, H] = [S^2, H] = 0$, where $S^2 = \frac{1}{2}(S^+S^- + S^-S^+) + (S^z)^2$ has the eigenvalue $S(S+1)$. The particle number $N = \sum_r (a_r^\dagger a_r + b_r^\dagger b_r) = N_\uparrow + N_\downarrow$ is conserved, and commutes with the Hamiltonian. Define the η-operators as follows: $\eta_r^+ = a_r^\dagger b_r^\dagger$, $\eta_r^- = b_r a_r$, $\eta_r^z = \frac{1}{2}(n_r - 1)$ with $n_r = n_r^a + n_r^b$, and $[\eta_r^+, \eta_{r'}^-] = 2\eta_r^z \delta_{r,r'}$, $[\eta_r^\pm, \eta_{r'}^z] = \mp \eta_r^\pm \delta_{r,r'}$. Below we will investigate the spin and the on-site pairing correlation functions of the model, and these definitions are necessary for subsequent analyses.

2.1. Symmetries of correlation functions

First let us for convenience write down three well-known unitary operators explicitly [3], which are frequently cited in the literature, and were usually applied for studying the transformed systems connected by them, but whose explicit forms are not obvious. The operator

$$\mathcal{U}_0 = \prod_r (b_r - \epsilon(r) b_r^\dagger)$$

with $\epsilon(r) = (-1)^r$ and $\mathcal{U}_0^\dagger \mathcal{U}_0 = 1$ describes the well-known particle–hole transformation [4]: $\mathcal{U}_0 a_r \mathcal{U}_0^\dagger = a_r, \mathcal{U}_0 b_r \mathcal{U}_0^\dagger = \epsilon(r) b_r^\dagger$, which makes $U_r \to -U_r$ in the Hamiltonian (2.1) with $\mu_r = U_r/2$ if $t_{r,r'} = -t$ for nearest neighbours and zero otherwise, like in the standard single-band Hubbard model. Here $(-1)^r$ can be understood as a factor $\mathrm{e}^{\mathrm{i}\boldsymbol{Q}\cdot\boldsymbol{r}}$ with $\boldsymbol{Q} = (\pi, \pi, \ldots)$ in two or three dimensions. The operator

$$\mathcal{U}_1 = \prod_r (a_r - a_r^\dagger)(b_r - b_r^\dagger)$$

with $\mathcal{U}_1^\dagger\mathcal{U}_1 = 1$ describes another symmetric particle–hole transformation: $\mathcal{U}_1 a_r \mathcal{U}_1^\dagger = a_r^\dagger, \mathcal{U}_1 b_r \mathcal{U}_1^\dagger = b_r^\dagger$ which makes $S_r^+ \to -S_r^-$, $S_r^z \to -S_r^z$, $\eta_r^+ \to -\eta_r^-$ and $t_{r,r'} \to -t_{r',r}$ in (2.1) with additional constants and proper adjustment of the chemical potential. The operator

$$\mathcal{U}_2 = \exp\left[\frac{\mathrm{i}\pi}{2}\sum_r (a_r^\dagger - b_r^\dagger)(a_r - b_r)\right]$$

with $\mathcal{U}_2^\dagger\mathcal{U}_2 = 1$ exchanges the spins (up–down symmetry): $\mathcal{U}_2 a_r^\dagger \mathcal{U}_2^\dagger = b_r^\dagger$, which leaves the Hamiltonian (2.1) unchanged, but makes $S_r^+ \to S_r^-$ and $S_r^z \to -S_r^z$. Of course, these unitary operators can be used either individually or in a combined way.

We now give some relations for thermal correlation functions. It is noteworthy that some of them are trivial, but some are less obvious and thus worth writing down. As the expectation value of the commutator, $[n_r^a, H] = \sum_{r'}(t_{r,r'}a_r^\dagger a_{r'} - t_{r',r}a_{r'}^\dagger a_r)$, vanishes, we get

$$\sum_{r'} t_{r,r'}\langle a_r^\dagger a_{r'}\rangle = \sum_{r'} t_{r',r}\langle a_{r'}^\dagger a_r\rangle \tag{2.2}$$

where $\langle\cdots\rangle$ denotes the thermal average. Using the up–down symmetry, connected by $\mathcal{U}_2$, we have

$$\sum_{r'} t_{r,r'}\langle b_r^\dagger b_{r'}\rangle = \sum_{r'} t_{r',r}\langle a_{r'}^\dagger a_r\rangle. \tag{2.3}$$

Note that (2.2) and (2.3) are general, not limited to the translation-invariant case, for we have not made use of any spatial symmetry of the lattice. The expectation value of the commutator $[S_{r'}^+ S_r^z, S^-] = 2S_{r'}^z S_r^z - S_{r'}^+ S_r^-$ yields

$$\langle S_{r'}^+ S_r^-\rangle = 2\langle S_{r'}^z S_r^z\rangle \tag{2.4}$$

due to S^- commuting with H. This symmetry is essential, for it is local, and is valid for any r and r'. Similarly, we can obtain a lot of such symmetries, for instance,

$$\begin{aligned}
&\langle S_{r'}^z S_r^\pm\rangle = 0 \qquad \langle S_r^\pm\rangle = \langle S_r^z\rangle = 0 \qquad \langle S_r^z n_{r'}\rangle = 0\\
&\langle S_{r'}^+ S_r^-\rangle = 2\langle n_r^a S_{r'}^z\rangle = -2\langle n_r^b S_{r'}^z\rangle \qquad \langle n_{r'}^a S_r^z\rangle = \langle n_r^a S_{r'}^z\rangle\\
&\langle S_{r'}^+ S_r^-\rangle = 2\langle S_r^z S_{r'}^+ S_{r'}^-\rangle = 2\langle S_r^+ S_r^- S_{r'}^z\rangle\\
&\langle n_{r'}^a n_r^b\rangle = \langle n_r^a n_{r'}^b\rangle \qquad \langle a_r b_r\rangle = \langle b_r^\dagger a_r^\dagger\rangle = 0\\
&\langle (S_r^z)^{2m+1}\rangle = 0
\end{aligned} \tag{2.5}$$

with $m = 1, 2, 3, \ldots$, etc. It can be seen that some of the above relations are obvious for the translation-invariant case, but less obvious for the system without translation invariance, and that these are probably useful for numerical calculations, and meanwhile give some restrictions on approximate methods. Moreover, one may apply the unitary transformations, as mentioned above, to equations (2.5), and can obtain the corresponding symmetries of correlation functions for the transformed systems. We will apply them below.

2.2. Magnetic correlation

Let us study the transverse spin correlation function $\langle S_{r'}^+ S_r^-\rangle$ for $r \neq r'$, which is related to the longitudinal correlation function through (2.4), by means of Bogoliubov's inequality [5]:

$$|\langle [A, B]\rangle|^2 \leqslant \frac{\beta}{2}\langle\{A, A^\dagger\}\rangle\langle[[B, H], B^\dagger]\rangle \tag{2.6}$$

with $\beta = T^{-1}$ ($k_B = 1$) the inverse temperature. Note that the relation between the spin correlation function and magnetic LRO was thoroughly established thirty years ago [6]. Since

$$[[S_r^z, H], S_r^z] = -\frac{1}{4}\sum_{r'(\neq r)}(t_{r',r}a_{r'}^\dagger a_r + t_{r,r'}a_r^\dagger a_{r'} + t_{r',r}b_{r'}^\dagger b_r + t_{r,r'}b_r^\dagger b_{r'})$$

we have

$$\langle[[S_r^z, H], S_r^z]\rangle = -\sum_{r'(\neq r)} t_{r,r'}\langle a_r^\dagger a_{r'}\rangle \geqslant 0 \tag{2.7}$$

where the non-negativity of (2.7) comes from the fact that the inner product $(B, B^*) \geqslant 0$ [5, 7]. By the Schwartz inequality $|\langle A^\dagger B\rangle| \leqslant \sqrt{\langle A^\dagger A\rangle\langle B^\dagger B\rangle}$ we observe that

$$\langle\{S_{r'}^+ S_r^-, S_r^+ S_{r'}^-\}\rangle \leqslant 8 \qquad (r' \neq r). \tag{2.8}$$

To obtain inequality (2.8) one has to substitute the definitions of spin operators into the left-hand side of (2.8), and then apply the Schwartz inequality to electron operators repeatedly by noting that $|\langle a_{r'}^\dagger a_r\rangle| \leqslant 1$ and $|\langle b_{r'}^\dagger b_r\rangle| \leqslant 1$. Therefore, setting $A = S_{r'}^+ S_r^-$ $(r \neq r')$ and $B = S_r^z$ in (2.6) and noticing (2.7) and (2.8), we get a bound

$$|\langle S_{r'}^+ S_r^-\rangle|^2 \leqslant -4\beta \sum_{r'(\neq r)} t_{r,r'}\langle a_r^\dagger a_{r'}\rangle \tag{2.9}$$

for $r' \neq r$. One may note that the index r' in the right-hand side (RHS) of (2.9) has been eliminated due to using the Schwartz inequality in (2.8). The same situation occurs in the following. Obviously, as $t_{r',r}(r' \neq r) \to 0$, then $|\langle S_{r'}^+ S_r^-\rangle| = 0$, which implies that there is no spin–spin correlation in the atomic limit, i.e., no magnetic (ferromagnetic and antiferromagnetic) LRO occurs in this case. One may notice that the RHS of inequality (2.9) depends only on the off-diagonal correlation function $\langle a_r^\dagger a_{r'}\rangle$ and hopping matrix element $t_{r,r'}$, independent of the local Coulomb potential U_r.

We define the operators

$$\alpha_{r,r'}^\dagger = t_{r',r}^{1/2} a_{r'} - t_{r,r'}^{1/2} a_r \qquad \alpha_{r,r'} = t_{r,r'}^{1/2} a_{r'}^\dagger - t_{r',r}^{1/2} a_r^\dagger. \tag{2.10}$$

Then $\langle\alpha_{r,r'}^\dagger \alpha_{r,r'}\rangle \geqslant 0$ gives

$$\sum_{r'(\neq r)} t_{r,r'}\langle a_r^\dagger a_{r'}\rangle \geqslant \frac{1}{2}\sum_{r'(\neq r)} |t_{r',r}|(\langle a_{r'}^\dagger a_{r'}\rangle + \langle a_r^\dagger a_r\rangle - 2). \tag{2.11}$$

Substituting (2.11) into (2.9) we have

$$|\langle S_{r'}^+ S_r^-\rangle|^2 \leqslant 2\beta \sum_{r'(\neq r)} |t_{r',r}|(2 - \langle a_{r'}^\dagger a_{r'}\rangle - \langle a_r^\dagger a_r\rangle). \tag{2.12}$$

If the system has translation invariance, then from (2.12) we verify rigorously the trivial fact that $|\langle S_{r'}^+ S_r^-\rangle| = 0$ for $r' \neq r$ at full filling. Although the bound (2.9) is lower than (2.12), sometimes the latter is also expected to be useful.

Since the RHS of (2.9) is intimately related to $\langle a_r^\dagger a_{r'}\rangle$, we now discuss it. For $r' \neq r$, we have $[a_r^\dagger a_{r'}, a_r^\dagger a_r] = -a_r^\dagger a_{r'}$. By setting $A = a_r^\dagger a_{r'}$ and $B = a_r^\dagger a_r$ in (2.6) one obtains

$$|\langle a_r^\dagger a_{r'}\rangle|^2 \leqslant -\beta\langle(n_r^a - n_{r'}^a)^2\rangle \sum_{r'(\neq r)} t_{r,r'}\langle a_r^\dagger a_{r'}\rangle \leqslant -2\beta \sum_{r'(\neq r)} t_{r,r'}\langle a_r^\dagger a_{r'}\rangle$$

for $r' \neq r$. This is a recursion inequality. It turns out to be

$$|\langle a_r^\dagger a_{r'}\rangle| \leqslant 2\beta \sum_{r'(\neq r)} |t_{r,r'}|. \tag{2.13}$$

Moreover, we are also able to obtain a bound

$$|\langle a_r^\dagger a_{r'}\rangle| \leqslant \sqrt{(\langle n_r^a\rangle - \langle n_r^a n_{r'}^a\rangle)(1-\langle n_r^a\rangle)} \tag{2.14}$$

for $r \neq r'$. The two bounds combined with (2.9) may help us to understand more about the spin correlation function.

Let us turn to a special case for the moment. Assume that $t_{r,r'} = -t$ with $t > 0$ for r, r' nearest neighbours, and $t = 0$ otherwise, like in the standard single-band Hubbard model but including the local Coulomb potential U_r. We introduce the Fourier transform of $a_r^\dagger$ as

$$a_r^\dagger = \frac{1}{\sqrt{M}}\sum_p a_p^\dagger \mathrm{e}^{-\mathrm{i}pr}$$

where the summation over p runs over the dual lattice defined by the boundary conditions. By summing over r ($\neq r'$) on both sides of (2.9) and inserting the Fourier transform into it we obtain

$$\sum_{r(\neq r')} |\langle S_{r'}^+ S_r^-\rangle|^2 \leqslant 2t\beta \sum_{p,\delta}\langle n_p\rangle \mathrm{e}^{\mathrm{i}p\delta}$$

where $|\delta|$ denotes the lattice spacing between nearest neighbours, and $n_p = a_p^\dagger a_p + b_p^\dagger b_p$. One may observe that when $\langle n_p\rangle = 1$ or constant, we have $|\langle S_{r'}^+ S_r^-\rangle| = 0$ for $r \neq r'$ because $\sum_p \mathrm{e}^{\mathrm{i}p\delta} = 0$. In other words, the single-band Hubbard model with a local Coulomb potential does not exhibit magnetic LRO at finite temperatures at $\langle n_p\rangle = 1$ or constant. This result is independent of the sign of U_r and for arbitrary dimensions. Although the condition $\langle n_p\rangle = 1$ or constant is very special, we rigorously rule out the possibility of magnetic LRO in this case.

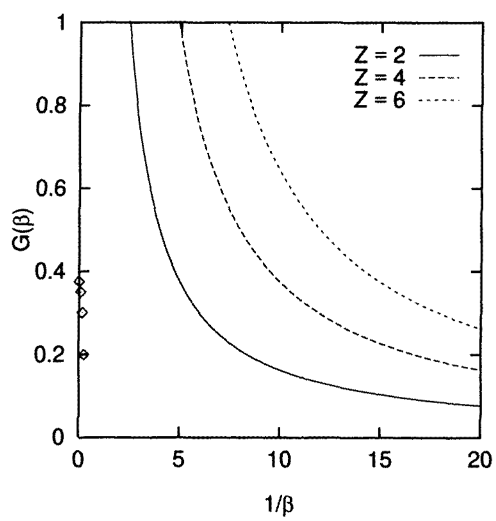

Figure 1. The temperature dependence of the bound (2.16), where β^{-1} is in units of $2t$, and coordinate numbers are taken as 6, 4, 2 respectively, as indicated. The numerical data are taken from [8].

If we do not bound $\langle\{S_{r'}^+ S_r^-, S_r^+ S_{r'}^-\}\rangle$ by the Schwartz inequality in (2.8), we have an expression

$$\langle S_{r'}^+ S_r^-\rangle \leqslant \frac{1}{2}\langle S_{r'}^+ S_{r'}^- S_r^+ S_r^-\rangle \tag{2.15}$$

where we have used (2.5) and $\langle\{A^\dagger, A\}\rangle \geqslant 0$. Then from (2.6) we get

$$|\langle S_{r'}^+ S_r^-\rangle| \leqslant \beta Q(r) + \sqrt{Q(r)^2\beta^2 + \beta P(r,r')Q(r)}$$

with $Q(r) = -\sum_{r'(\neq r)} t_{r,r'}\langle a_r^\dagger a_{r'}\rangle$ and $P(r, r') = |\langle S_{r'}^+ S_{r'}^- S_r^+ S_r^-\rangle| \leqslant 1$ for $r \neq r'$. By noting (2.13) we can obtain an upper bound for the spin–spin correlation function:

$$|\langle S_{r'}^+ S_r^-\rangle| \leqslant G(\beta) = 2\beta^2 R(r) + \sqrt{4\beta^4 R(r)^2 + 2\beta^2 R(r)} \tag{2.16}$$

with $R(r) = (\sum_{r'(\neq r)} |t_{r,r'}|)^2$. To define the bound unambiguously, we assume that $t_{r,r'} = t$ for r, r' nearest neighbours and 0 otherwise. We plot $G(\beta)$ versus temperature β^{-1}, as shown in figure 1, where β^{-1} is in units of $2t$, and the coordinate numbers are taken as $6, 4, 2$, respectively. Since $|\langle S_{r'}^+ S_r^-\rangle| \leqslant 1$, we only plot the interesting part. From figure 1 one may see that the bound decreases rapidly with increasing temperature. When $\beta^{-1} > 20$, the bound decreases slowly, eventually to zero, as temperature increases. Evidently, the decay of the spin–spin correlation function with temperature cannot be slower than the inverse square law at low temperatures and the inverse law at high temperatures. Although the bound as well as the bound (2.12) cannot tell us in general whether the system can exhibit magnetic LRO or not, it may shed useful light on the validity of some kinds of approximation and numerical result, especially regarding the temperature dependence of spin–spin correlation functions. We note that the spin–spin correlation function of the single-band Hubbard model was studied numerically for small sizes (4×4) of a square lattice at half-filling at low temperatures [8]. The calculated results are found to be smaller than the present bound, as indicated in figure 1. The reason for this discrepancy may be that in spite of the finite-size effects in numerical calculations, the present bound is suitable for macroscopic sizes of lattices and is better for high temperatures.

2.3. Pairing correlation

To investigate the on-site superconducting correlation, we need to calculate the on-site pairing correlator $\langle \eta_r^+ \eta_{r'}^-\rangle = \langle a_r^\dagger b_r^\dagger b_{r'} a_{r'}\rangle$ in the off-diagonal long-range (ODLR) limit [9] $|r - r'| \to \infty$, namely, for off-diagonal long-range order (ODLRO) [10]. As before, we use Bogoliubov's inequality. Choosing $A = \eta_r^+ \eta_{r'}^-$ and $B = \eta_r^z$ in (2.6), and noticing that $[\eta_r^+ \eta_{r'}^-, \eta_r^z] = -\eta_r^+ \eta_{r'}^-$ for $r \neq r'$, and

$$\langle [[\eta_r^z, H], \eta_r^z]\rangle = -\sum_{r'(\neq r)} t_{r',r}\langle a_{r'}^\dagger a_r\rangle \tag{2.17}$$

we have the bound

$$|\langle \eta_r^+ \eta_{r'}^-\rangle|^2 \leqslant -\beta \sum_{r'(\neq r)} t_{r',r}\langle a_{r'}^\dagger a_r\rangle \tag{2.18}$$

where we have used the Schwartz inequality to obtain the bound $\langle\{\eta_r^+ \eta_{r'}^-, \eta_{r'}^+ \eta_r^-\}\rangle \leqslant 2$. One may observe that if $t_{r,r'} \to 0$, then $|\langle \eta_r^+ \eta_{r'}^-\rangle| \to 0$. This suggests that no on-site pairing correlation in the general Hubbard model exists in the atomic limit.

Since

$$\sum_{r,r'(r\neq r')} \langle a_{r'}^\dagger a_r\rangle = \sum_{r,r'} \langle a_{r'}^\dagger a_r\rangle - N_\uparrow = M\langle n_0^a\rangle - N_\uparrow \tag{2.19}$$

with $\langle n_0^a\rangle = \langle a_0^\dagger a_0\rangle$ the number density with zero momentum of spin-up electrons, and further assuming that $t_{r',r} \equiv t =$ constant, from (2.18) one obtains

$$\frac{1}{M}\sum_r |\langle \eta_r^+ \eta_{r'}^-\rangle|^2 \leqslant -\frac{\beta t}{2}(\langle n_0\rangle - \rho) \tag{2.20}$$

with $\langle n_0\rangle = \langle a_0^\dagger a_0 + b_0^\dagger b_0\rangle$ and $\rho = \sum_r \langle n_r\rangle / M$. We note that if $t > 0$ and $\langle n_0\rangle \geqslant \rho$ or $t < 0$ and $\langle n_0\rangle \leqslant \rho$, then $|\langle a_r^\dagger b_r^\dagger b_{r'} a_{r'}\rangle| = 0$ for $r \neq r'$ from (2.20). In other words, the system cannot exhibit the on-site pairing condensation in the aforementioned circumstances. From the derivation, one may note that the electron hopping terms play a key role in pairing condensation phenomena in itinerant-electron systems. Besides, this one may observe that the sign of t also has an effect on the final result, as shown above. Of course, this argument can also apply to (2.9).

If we exchange A and B in the derivation of (2.18), then we can get $|\langle\eta_r^+\eta_{r'}^-\rangle|^2 \leqslant \beta\langle(\eta_r^z)^2\rangle\langle[[B, H], B^\dagger]\rangle$. One may see that if

$$\langle n_r^a n_r^b\rangle \leqslant \tfrac{1}{2}(\langle n_r\rangle - 1) \tag{2.21}$$

we have $|\langle\eta_r^+\eta_{r'}^-\rangle| = 0$. That is, under the condition of (2.21), the Hubbard model cannot show the on-site pairing condensation at finite temperatures. Condition (2.21) is not anomalous; e.g., the case of half-filling with $\langle n_r^a n_r^b\rangle = 0$ obeys it.

If $t_{r,r'} = -t$ for r, r' nearest neighbours and/or next-nearest neighbours and 0 otherwise, then—similarly to in discussions of spin correlation functions—we also have $|\langle a_r^\dagger b_r^\dagger b_{r'} a_{r'}\rangle| = 0$ for $r \neq r'$ at $\langle n_p\rangle = 1$. We notice that Veilleux *et al* [11] have recently studied the pair correlations of the Hubbard model with next-nearest-neighbour hopping by using the quantum Monto Carlo method. The consequences that they derive are qualitatively in agreement with the present rigorous result in the parameter region that they studied.

By substituting (2.13) into (2.18), we get a rigorous upper bound for the off-diagonal element of the two-particle reduced density matrix:

$$|\langle a_r^\dagger b_r^\dagger b_{r'} a_{r'}\rangle| \leqslant \sqrt{2}\beta \sum_{r'(\neq r)} |t_{r',r}| \tag{2.22}$$

which should also be valid in the limit $|r - r'| \to \infty$. This bound suggests that the decay of ODLRO with temperature is not slower than the inverse law. Although the bound is too loose to compare with the numerical data on small clusters at low temperatures [8], it gives a hint as regards the pairing correlation function in the thermodynamic limit. Since $\langle a_r^\dagger b_r^\dagger b_{r'} a_{r'}\rangle$ is related to the superconducting order parameter $\langle a_r b_r\rangle$ (quasi-average) by the asymptotic property [12] $\langle a_r^\dagger b_r^\dagger b_{r'} a_{r'}\rangle \to |\langle a_r b_r\rangle|^2$ in the ODLR limit, equation (2.22) provides a standard for approximants in calculating the temperature dependence of the pairing order parameter. Here we would like to point out that one may obtain bounds similar to (2.22) for other pairings—for instance, the extended s wave and d wave [13].

3. The t–J model

This model has been extensively studied in recent years, but rigorous results are rare, except that the one-dimensional (1D) supersymmetric model ($J = \pm 2t$) can be exactly solved using the Bethe *ansatz* [14]. Many approximate or numerical results on magnetic and pairing correlations in high dimensions in this model differ quite strongly [8]. We study the following Hamiltonian:

$$H_{t-J} = -t \sum_{\langle r,r'\rangle} (a_r^\dagger a_{r'} + b_r^\dagger b_{r'}) + J \sum_{\langle r,r'\rangle} \left(\boldsymbol{S}_r \cdot \boldsymbol{S}_{r'} - \frac{1}{4} n_r n_{r'} \right) \tag{3.1}$$

on a d-dimensional lattice, where the notation is the same as in section 2, $\langle r, r'\rangle$ are nearest neighbours, $J > 0$ (we here consider J, without loss of the generality, as an independent parameter), and $t > 0$. The different forms of the model have been discussed elsewhere [15]. In this model, we assume that double occupancy of every site is excluded. In other words, each lattice site is constrained to have either one electron (with spin up or down) or none, as usual. It can be seen that the system has SU(2) spin symmetry. We may also obtain some symmetries of correlation functions as in section 2. In this section we will first derive an upper bound for the average energy, then study the spin–spin correlation function, and finally discuss the nearest-neighbour pairing correlation function.

3.1. The upper bound for the average energy

From (3.1) we find

$$\langle[[S_r^+, H_{t-J}], S_r^-]\rangle = t\sum_{r'_{\langle r\rangle}}\langle a_{r'}^\dagger a_r + b_r^\dagger b_{r'}\rangle - 2J\sum_{r'_{\langle r\rangle}}\langle 2S_r^z S_{r'}^z + S_{r'}^+ S_r^-\rangle \tag{3.2}$$

where $r'_{\langle r\rangle}$ denotes the summation on r' running over nearest neighbours of r. Equation (3.2) then implies

$$\sum_{r'_{\langle r\rangle}}\langle S_{r'}^+ S_r^-\rangle \leqslant \frac{t}{4J}\sum_{r'_{\langle r\rangle}}\langle a_{r'}^\dagger a_r + b_r^\dagger b_{r'}\rangle \tag{3.3}$$

where we have used (2.4) and the non-negative property [5, 7] of (3.2). By noting (3.3) and $\langle S_r^+ S_{r'}^-\rangle = \langle S_{r'}^+ S_r^-\rangle$ one gets

$$\langle H_{t-J}\rangle \leqslant -\frac{5}{8}t\sum_{\delta,p}\langle n_p\rangle e^{ip\delta} - \frac{J}{4}\sum_{\langle r,r'\rangle}\langle n_r n_{r'}\rangle.$$

At temperature T, we have the average energy (internal energy) $E_0 = \langle H_{t-J}\rangle$. On the other hand, the non-negativity of $\langle[[a_r b_r, H_{t-J}], b_r^\dagger a_r^\dagger]\rangle$ yields

$$-t\sum_{\langle r,r'\rangle}\langle a_r^\dagger a_{r'} + b_r^\dagger b_{r'}\rangle \leqslant \frac{J}{2}\sum_{\langle r,r'\rangle}\langle n_r n_{r'}\rangle - \frac{J}{2}Nz$$

with z the coordinate number, and thus

$$E_0 \leqslant \frac{J}{16}\sum_{\langle r,r'\rangle}\langle n_r n_{r'}\rangle - \frac{5J}{16}Nz.$$

Furthermore, since $\langle(n_r - n_{r'})^2\rangle \geqslant 0$ and noting that $\langle n_r^a n_r^b\rangle = 0$ due to the restriction of no doubly occupied sites, one has $\langle n_r n_{r'}\rangle \leqslant \frac{1}{2}(\langle n_r\rangle + \langle n_{r'}\rangle)$. Substituting these results into E_0 we have

$$E_0 \leqslant -\tfrac{1}{4}JzN. \tag{3.4}$$

We would like to point out that the bound (3.4) is generic, not limited to the translation-invariant system, and is valid for arbitrary filling fraction and arbitrary dimensions. If the system has the singlet ground-state, then E_0 at $T \to 0$ can be regarded as the ground-state energy, and $\langle\cdots\rangle$ thus means the average in the ground state. If the ground state of the system is degenerate, E_0 can also be understood as the ground-state energy for all ground states. At half-filling, the t–J model reduces to the Heisenberg antiferromagnetic model. In 1D the ground-state energy is well known to be $E_0/M = -J\ln 2$ [14], which clearly satisfies (3.4): $E_0/M = -0.693\,147\,J < -0.5J$. Away from half-filling, the ground-state energy of the supersymmetric t–J model also complies with the bound (3.4), as shown in [14, 18]. In 2D, the numerical result for estimating the ground-state energy of one hole in the interval $0.2 \leqslant J/t \leqslant 1.0$ for small clusters (4×4) is $E_0/M = -3.17t + 2.83t(J/t)^{0.73}$ [16]. However, the Hamiltonian from [14] does not contain the term $-(J/4)\sum_{\langle r,r'\rangle} n_r n_{r'}$. If this term is taken into account, the numerical results of [14] would be in agreement with the present bound. Since this bound is a rigorous result, it can be expected to provide checks for approximate and numerical methods, especially in high dimensions.

3.2. Magnetic correlation

The magnetic structure factor $m(p)$ is given by

$$m(p) = \frac{1}{M}\sum_{r,r'} \mathrm{e}^{\mathrm{i}p(r-r')}\langle S_r^z S_{r'}^z\rangle = \langle S_p^z S_{-p}^z\rangle \tag{3.5}$$

where $S_p^z = (1/\sqrt{M})\sum_r S_r^z \mathrm{e}^{\mathrm{i}pr}$. By symmetry, $\langle S_p^z S_{-p}^z\rangle = \frac{1}{2}\langle S_p^+ S_p^-\rangle$. From (3.3) we obtain

$$\sum_p \left[m(p) - \frac{t}{8J}\langle n_p\rangle\right]\gamma_p \leqslant 0 \tag{3.6}$$

with $\gamma_p = \sum_\delta \mathrm{e}^{\mathrm{i}p\delta}$. Note that $m(p) \geqslant 0$. Inequality (3.6) imposes a severe restriction on $m(p)$ in the t–J model. If $\langle n_p\rangle = 1$ or $t = 0$, we have $\sum_p m(p)\gamma_p \leqslant 0$. Since the existence of Néel order corresponds to $m(p)$ containing a δ-function at $\boldsymbol{Q} = (\pi, \pi, \ldots)$ in the infinite-volume limit [17], and letting m^2 be the coefficient of this δ-function, we get from (3.6) a bound

$$m^2\gamma_Q \leqslant \frac{t}{8J}\sum_p \langle n_p\rangle\gamma_p - \sum_{p\neq Q} m(p)\gamma_p. \tag{3.7}$$

It has been shown that the 3D half-filled t–J model, i.e., the Heisenberg antiferromagnetic model, exhibits LRO [17]. Away from half-filling, equation (3.7) may shed some light on the antiferromagnetic order of the t–J model. For a square lattice, $\gamma_Q = -4$. Then we have

$$m^2 \geqslant \frac{1}{4}\sum_{p\neq Q} m(p)\gamma_p - \frac{t}{32J}\sum_p \langle n_p\rangle\gamma_p.$$

If we obtain a bound for $\sum_{p\neq Q} m(p)\gamma_p$, then we can say something about the antiferromagnetic LRO in the model, which will be left for future study.

We choose $A = S_{r'}^- S_r^z$ and $B = S_r^+$ in (2.6). Then $[A, B] = S_{r'}^- S_r^z$ for $r \neq r'$. Since $\frac{1}{2}\langle\{S_{r'}^- S_r^z, S_r^z S_{r'}^+\}\rangle \leqslant \frac{1}{4}$ by the Schwartz inequality, from (2.6) and (3.2) we have

$$|\langle S_{r'}^+ S_r^-\rangle| \leqslant \sqrt{\frac{\beta}{8}\left(t\sum_{r'_{\langle r\rangle}}\langle a_{r'}^\dagger a_r + b_r^\dagger b_{r'}\rangle - 4J\sum_{r'_{\langle r\rangle}}\langle S_{r'}^+ S_r^-\rangle\right)}$$

$$\leqslant \sqrt{\frac{z\beta}{4}\left(t + 2J\sqrt{\frac{z\beta}{4}\left(t + 2J\sqrt{\frac{z\beta}{4}(t + 2J\sqrt{\cdots})}\right)}\right)}. \tag{3.8}$$

This inequality gives an upper bound for the spin–spin correlation function in the t–J model. In particular, as $t = 0$, the model reduces to the Heisenberg antiferromagnetic model, and (3.8) becomes

$$|\langle S_{r'}^+ S_r^-\rangle| \leqslant (J\beta/2)z. \tag{3.9}$$

That is, the temperature dependence of the spin–spin correlation function cannot be slower than the inverse law in the Heisenberg antiferromagnetic model.

3.3. Pairing correlation

Now we come to discussing the pairing correlation function. Since there are no doubly occupied sites in the system, the on-site pairing correlation should be vanishing. In the following we consider the nearest-neighbour pairing order parameter $\langle a_{r_1} b_{r_2}\rangle$ with r_1, r_2

being nearest-neighbour sites. For this purpose, we have to add a U(1) symmetry-breaking term $H' = -\alpha\sum_{\langle r_1,r_2\rangle}(a_{r_1}b_{r_2} + b^\dagger_{r_2}a^\dagger_{r_1})$ as well as the chemical potential term $-\mu\sum_r n_r$ into the Hamiltonian H_{t-J}. Let $B = a_{r_1}b_{r_2}$, and $A = a^\dagger_{r_1}a_{r_1} + b^\dagger_{r_2}b_{r_2}$. Then

$$[A, B] = -2a_{r_1}b_{r_2} \qquad \langle[[a_{r_1}b_{r_2}, H_{t-J}], b^\dagger_{r_2}a^\dagger_{r_1}]\rangle \leqslant D(r_1, r_2)$$

with

$$D(r_1, r_2) = t\left(\sum_{r_{\langle r_1\rangle}}\langle a^\dagger_{r_1}a_r\rangle + \sum_{r_{\langle r_2\rangle}}\langle b^\dagger_{r_2}b_r\rangle\right) - (J + 2\mu)(1 - \langle n^a_{r_1}\rangle - \langle n^b_{r_2}\rangle) + 2J\langle n^a_{r_1}n^b_{r_2}\rangle + 6Jz - \alpha\left(\sum_{r_{\langle r_2\rangle}} a^\dagger_r b^\dagger_{r_2} + \sum_{r_{\langle r_1\rangle}} b^\dagger_r a^\dagger_{r_1}\right)$$

and $\langle\{A, A^\dagger\}\rangle \leqslant 8$. Substituting these results into (2.6) we obtain the bound

$$|\langle a_{r_1}b_{r_2}\rangle|^2 \leqslant \beta D(r_1, r_2) \tag{3.10}$$

as $\alpha \to 0$ in the thermodynamic limit, where we have used the Schwartz inequality to bound those terms with four creation and annihilation operators. One may note that $\langle a_{r_1}b_{r_2}\rangle$ in (3.10) is Bogoliubov's quasi-average [12]. On the other hand, according to Bogoliubov's argument [12], the off-diagonal element of the two-particle reduced density matrix $\langle b^\dagger_{r'_2}a^\dagger_{r'_1}a_{r_1}b_{r_2}\rangle$ has the asymptotic behaviour

$$\langle b^\dagger_{r'_2}a^\dagger_{r'_1}a_{r_1}b_{r_2}\rangle \to \langle b^\dagger_{r'_2}a^\dagger_{r'_1}\rangle\langle a_{r_1}b_{r_2}\rangle \tag{3.11}$$

in the ODLR limit [13] $|(r'_2, r'_1) - (r_2, r_1)| \to \infty$. It is worth mentioning that (3.11) is not incompatible with Haag's spatial cluster theorem [19]. In the translation-invariant system, the temperature dependence of ODLRO should thus obey

$$\langle b^\dagger_0 a^\dagger_1 a_{r_1}b_{r_2}\rangle \leqslant \beta D(r_1, r_2) \tag{3.12}$$

i.e., the decay of the ODLRO for nearest-neighbour pairs with temperature in the t–J model with translation invariance cannot be slower than the inverse law. This bound thus offers a check for some approximate results on the temperature dependence of the superconducting order parameter.

4. The Hubbard model with bond–charge interaction

The Hamiltonian of the model is given by

$$H_{b-c} = -t\sum_{\langle r,r'\rangle}(a^\dagger_r a_{r'} + b^\dagger_r b_{r'} + \mathrm{HC}) + U\sum_r a^\dagger_r a_r b^\dagger_r b_r + X\sum_{\langle r,r'\rangle}[(a^\dagger_r a_{r'} + \mathrm{HC})(n^b_r + n^b_{r'}) + (b^\dagger_r b_{r'} + \mathrm{HC})(n^a_r + n^a_{r'})] - \mu\sum_r(a^\dagger_r a_r + b^\dagger_r b_r) \tag{4.1}$$

where X is the bond–charge interaction, and the other notation is standard, as usual. This model has been extensively discussed by Hirsch [20], Bariev *et al* [21], de Boer *et al* [22] and Schadschneider [23]. It has been shown [22] that the η-pairing state with ODLRO is the ground state if $U \leqslant -2Z|t|$, and can be solved exactly in one dimension [21–23], as $t = X$ and $\mu = U/2$. For certain values of X and large densities of electrons (small doping) the bond–charge interaction may lead to an attractive effective interaction between the holes within the framework of BCS mean-field theory [20]. In this section, we will give a few rigorous bounds for the spin–spin and the on-site pairing correlation functions of this system.

As in the method exploited in preceding sections, it is not difficult to obtain the following two bounds:

$$|\langle S_r^+ S_{r'}^- \rangle| \leqslant \left[8\beta \left(t \sum_{r'_{\langle r \rangle}} \langle a_{r'}^\dagger a_r \rangle - X \sum_{r'_{\langle r \rangle}} \langle a_{r'}^\dagger a_r (n_r^b + n_{r'}^b) \rangle \right) \right]^{1/2} \tag{4.2}$$

$$|\langle a_r^\dagger b_r^\dagger b_{r'} a_{r'} \rangle| \leqslant \left[2\beta \left(t \sum_{r'_{\langle r \rangle}} \langle a_{r'}^\dagger a_r \rangle - X \sum_{r'_{\langle r \rangle}} \langle a_{r'}^\dagger a_r (n_r^b + n_{r'}^b) \rangle \right) \right]^{1/2} \tag{4.3}$$

for $r \neq r'$ by setting $A = S_r^+ S_{r'}^-$ and $\eta_r^+ \eta_{r'}^-$ with $r \neq r'$ and $B = S_r^z$ and η_r^z in (2.6), respectively, where we have used the spin-flip symmetry ($\mathcal{U}_2$). Evidently, if X satisfies the following condition:

$$X \sum_{r'_{\langle r \rangle}} \langle a_{r'}^\dagger a_r (n_r^b + n_{r'}^b) \rangle \geqslant t \sum_{r'_{\langle r \rangle}} \langle a_{r'}^\dagger a_r \rangle \tag{4.4}$$

then there is no spin–spin correlation or on-site pairing correlation. To ensure the existence of magnetism and superconductivity in the system H_{b-c}, the condition opposite to inequality (4.4) must hold, which gives a restriction on the values of X.

For the special case where $t = X$, the system possesses symmetric particle–hole symmetry, connected by the unitary operator $\mathcal{U}_1$, as discussed in [23], the η-pairing symmetry [22] at half-filling, and so forth. This model is very interesting, and the details will be presented in a separate publication.

5. Summary

We have rigorously investigated magnetic and superconducting pairing correlation functions in a general class of Hubbard models, the t–J model and a single-band Hubbard model with additional bond–charge interaction by means of Bogoliubov's inequality. Some corresponding upper bounds are obtained, which are expected to provide certain checks and standards for approximate methods. In some special cases, these bounds rule out the possibility of corresponding magnetic and pairing LRO.

For the Hubbard models, we obtained an upper bound for the spin–spin correlation function, which indicates that the decay of the correlation function with temperature cannot be slower than the inverse square law at low temperatures and the inverse law at high temperatures. From these bounds we observe that there is no magnetic LRO in the atomic limit and in the case with the momentum distribution function being constant for the model with only nearest-neighbour hopping. An upper bound for the on-site pairing correlation function was obtained, which suggests that the decay of the on-site pairing ODLRO with temperature is not slower than the inverse law. Since our method is rigorous, the present result may be applied for clarifying some contradictions in approximate calculations. In addition, we found that there is no on-site pairing correlation in the atomic limit and in the cases of either (i) $t > 0$ and $\langle n_0 \rangle \geqslant \rho$ or $t < 0$ and $\langle n_0 \rangle \leqslant \rho$ (see (2.20)) or (ii) $\langle n_p \rangle$ being constants for the single-band model but with local Coulomb interaction. It is emphasized that all of the bounds obtained are independent of the local on-site Coulomb interaction and are valid for arbitrary dimensions.

For the t–J model, we obtained an upper bound for the average energy (internal energy) for arbitrary electron fillings. Whatever the ground state of the system is, unique or not, the upper bound for $T \to 0$ can be regarded as that of the ground-state energy. Since the bound is rigorous, it provides a standard for approximate and numerical methods. We also obtained a lower bound for the Néel order, which may shed useful light on the antiferromagnetic order of the system. An upper bound for the spin–spin correlation function was derived, which implies that the decay of this function with temperature in the model is not slower than the $\beta^{1/2}$-law away from half-filling and the inverse law at half-filling. An upper bound for the nearest-neighbour pairing correlation was obtained for the translation-invariant system, which suggests that the decay of ODLRO with temperature cannot be slower than the inverse law. The results hold for arbitrary dimensions.

For the Hubbard model with bond–charge interaction, we obtained two bounds for the spin–spin correlation function and the on-site pairing correlation function, which impose severe restrictions on the values of the bond–charge interaction.

Acknowledgments

The author has benefited from discussions with Dr A Schadschneider and Professor B H Zhao. He is also grateful to Professor J Zittartz, Dr A Klümper and the ITP of the Universität zu Köln for warm hospitality. This work was supported by the Alexander von Humboldt Stiftung.

References

[1] Anderson P W 1987 *Science* **235** 1196
Zhang F C and Rice T M 1988 *Phys. Rev.* B **37** 3759
[2] See
M Rasetti (ed) 1991 *The Hubbard Model: Recent Results* (Singapore: World Scientific)
Lieb E H 1995 *Proc. Conf. Advances in Dynamical Systems and Quantum Physics* ed V Figari *et al* (Singapore: World Scientific) pp 173–93
Strack R and Vollhardt D 1995 *J. Low Temp. Phys.* **99** 385
[3] Yang C N and Zhang S C 1990 *Mod. Phys. Lett.* B **4** 759
[4] Pu F C and Shen S Q 1994 *Phys. Rev.* B **50** 16 086
[5] Mermin N D and Wagner H 1966 *Phys. Rev. Lett.* **17** 1133
Ghosh D K 1971 *Phys. Rev. Lett.* **27** 1584
[6] Griffiths R 1966 *Phys. Rev.* **152** 240
[7] Dyson F J, Lieb E H and Simon B 1978 *J. Stat. Phys.* **18** 335
[8] Dagotto E 1994 *Rev. Mod. Phys.* **66** 763 and references therein
[9] Nieh H T, Su G and Zhao B H 1995 *Phys. Rev.* B **51** 3076
[10] Yang C N 1962 *Rev. Mod. Phys.* **34** 694
[11] Veilleux A F, Dáre A, Chen L, Vilk Y and Tremblay A 1995 *Phys. Rev.* B **52** 16 255
[12] Bogoliubov N N 1960 *Physica* **26** S1
[13] Van Harlingen D J 1995 *Rev. Mod. Phys.* **67** 515
[14] Schlottman P 1987 *Phys. Rev.* B **36** 5177
Bares P A and Blatter G 1990 *Phys. Rev. Lett.* **64** 2567
[15] Su G 1993 *J. Phys. A: Math. Gen.* **26** L139
[16] Dagotto E, Moreo A, Joynt R, Bacci S and Gagliano E 1990 *Phys. Rev.* B **41** 2585
[17] Kennedy T, Lieb E H and Shastry B S 1988 *J. Stat. Phys.* **53** 1019
[18] Kawakami N and Yang S-K 1991 *J. Phys.: Condens. Matter* **3** 5983
[19] Haag R 1992 *Local Quantum Physics* (Berlin: Springer)
[20] Hirsch J E 1989 *Phys. Lett.* **134A** 451; 1991 *Phys. Rev.* B **43** 11 400
[21] Bariev R Z, Klümper A, Schadschneider A and Zittartz J 1993 *J. Phys. A: Math. Gen.* **26** 1249, 4863
[22] de Boer J, Korepin V E and Schadschneider A 1995 *Phys. Rev. Lett.* **74** 789
de Boer J and Schadschneider A 1995 *Phys. Rev. Lett.* **75** 4298
[23] Schadschneider A 1995 *Phys. Rev.* B **51** 10 386 and references therein