Vol 18 No 6, June 2009
1674-1056/2009/18(06)/2475-06

Chinese Physics B

© 2009 Chin. Phys. Soc.
and IOP Publishing Ltd

Single-particle spectral function of the Hubbard chain: frustration induced*

Wang Jing(王 竞)[a)b)†] and Enrico Arrigoni[b)]

[a)] *Department of Physics, Fudan University, Shanghai* 200433, *China*

[b)] *Institute of Theoretical Physics and Computational Physics, Graz University of Technology, A*-8010 *Graz, Austria*

(Received 16 December 2008; revised manuscript received 9 January 2009)

The one-electron spectral function of a frustrated Hubbard chain is computed by making use of the cluster perturbation theory. The spectral weight we found turns out to be strongly dependent on the frustrating next-nearest-neighbor hopping t'. A frustration induced pseudogap arises when the system evolves from a gapful Mott insulator to a gapless conductor for an intermediate value of the frustration parameter $|t'|$. Furthermore, the opening of a pseudogap in the density of states already in the metallic side leads to a continuous opening of the true gap in the insulator. For the hole-doped case, the pseudogap is pinned at the Fermi energy, while the Mott gap is shifted in energy with increasing Hubbard interaction U. The separation of the pseudogap and Mott gap in the hole-doped system demonstrates the validity of the existence of a pseudogap.

Keywords: cluster perturbation theory, pseudogap, metal-insulator transitions
PACC: 7110F, 7127, 7130, 9265H

1. Introduction

The observation of the pseudogap (PG) phenomenon in high-T_c superconductors via a number of experimental techniques, including angle-resolved photoemission spectroscopy (ARPES),[1] transport measurement,[2] neutron scattering,[3] and specific heat measurements,[4] has drawn much attention among scientists. It is believed that a better understanding of this phenomenon could lead to a better comprehension of the physics of the high-T_c materials.[5−10] Several experimental studies proved the existence of a pseudogap phase in several high-T_c superconductors,[11−17] and observed the persistence of this phase at low temperatures.[18−20] It has been observed that the PG shows up differently in the samples depending on whether the system is doped with holes or electrons.

A Hubbard chain with nearest-neighbor hopping t and next-nearest-neighbor hopping (frustration hopping) t' can be used to describe some properties of low-dimensional strongly correlated cuprate materials. For example, the model has been successfully used to study double-chain materials like $SrCuO_2$[21] or LiV_2O_5,[22] where the frustration hopping is expected to be substantial. When the next-nearest-neighbor coupling is turned off ($t' = 0$), the model returns to the extensively used standard one-dimensional (1D) Hubbard chain. In which, spin-charge separation is observed in its single-particle spectrum.[23] When t' is turned on, the system becomes frustrated, and its physics is quite different from the unfrustrated 1D Hubbard model.

Several theoretical works for the frustrated 1D Hubbard model[24−29] have shown that the frustration t' induces new properties in strongly correlated systems. Recently, Daul *et al* illustrated, by means of the density-matrix renormalization group technique, the existence of a rich ground-state phase diagram.[24] Hamacher *et al* observed different renormalizations of different Fermi wave vectors due to electron-electron correlations in such models.[25] The single-particle spectral function provides important information about the properties of strongly correlated electronic systems, as it is directly related to the data from ARPES measurements.[17,18] Several methods have been used in order to evaluate the spectral weight on models for strongly-correlated systems

*Project partly supported by the National Natural Science Foundation of China, the Ministry of Science and Technology of China (Grant No 2006CB921302), by the EC Project OFSPIN (Grant No NMP3-CT-2006-033370), by the Austrian Science Fund (Grant No FWF P18551-N16), and by the Eurasia Pacific Uninet.

†E-mail: jwang_80@fudan.edu.cn

and to study the properties of the PG state.[30−34] Many works have focused on the application to quasi-one-dimensional systems.[35] In this work, we study the frustration induced PG in a one-dimensional (1D) Hubbard chain by a numerical study of the single-particle spectral function with the method of cluster perturbation theory (CPT).[36,37] Our goal is to analyze the contribution of the frustration hopping to the spectral function and to discuss the frustration-induced PG at half filling and at finite doping within the frustrated Hubbard chain model.

The rest of the paper is organized as follows. In Section 2, the frustrated Hubbard chain and the CPT approach we used in this work are described. In Section 3, we present our numerical results and make a detailed discussion based on these results. We give a brief summary of this work in the last section.

2. Model and computational method

The model is described by the Hubbard Hamiltonian

$$\begin{aligned} H = & -t\sum_{i\sigma}(c^{\dagger}_{i+1\sigma}c_{i\sigma} + \text{H.c}) \\ & - t'\sum_{i\sigma}(c^{\dagger}_{i+2\sigma}c_{i\sigma} + \text{H.c.}) \\ & + U\sum_{i} n_{i\uparrow}n_{i\downarrow}, \end{aligned} \tag{1}$$

where $c^{\dagger}_{i,\sigma}$ ($c_{i,\sigma}$) is the electron creation (destruction) operator with spin σ at the i-th site, $n_{i\sigma}$ is the corresponding number operator, U is the on-site Coulomb interaction, t (t') is the nearest-neighbor (next-nearest-neighbor) hopping. We use the CPT to calculate the single-particle spectral function. Within CPT[37] the original lattice is first divided into disconnected clusters with the same size, and the exact diagonalization (ED) method is applied to calculate the Green's function of the unit cluster. We divide the lattice into identical clusters with N_c sites each. The Green's function of a single cluster is evaluated as

$$\begin{aligned} G^{c}_{i,j}(\omega) = & \langle\phi_0|c_i\frac{1}{\omega-(H-E_0)}c^{\dagger}_j|\phi_0\rangle \\ & + \langle\phi_0|c^{\dagger}_j\frac{1}{\omega+(H-E_0)}c_i|\phi_0\rangle \end{aligned} \tag{2}$$

by means of the usual Lanczos method.[38] Here, ω is a complex frequency, and E_0 is the energy of the ground state $|\phi_0\rangle$ of a cluster. $G^c(\omega)$ is an $N_c \times N_c$ matrix in the cluster-site indices, and the two terms in Eq. (2) describe creation and destruction of one electron from the ground state $|\phi_0\rangle$, respectively. The approximation now consists in extending the cluster results to the infinite lattice by treating the hopping between clusters in strong-coupling perturbation theory. Within this approximation, the single-particle Green's function of the lattice is written in the form

$$G_{i,j}(k,\omega) = \left(\frac{G^c(\omega)}{1-V(K)G^c(\omega)}\right)_{i,j}, \tag{3}$$

where $V(K)$ is the Fourier transformation of the $N_c \times N_c$ hopping matrix which is non-zero only for hopping processes across the cluster boundaries, K is a vector of the reduced Brillouin zone associated to cluster superlattice. The Green's function of Eq.(3) is in a mixed representation: real space for cluster sites and Fourier space between clusters. The single-particle spectral function $A(k,\omega)$ is obtained from the Green's function $G(k,\omega)$ as

$$A(k,\omega) = -\frac{1}{\pi}\text{Im}\,G(k,\omega+\text{i}\eta), \tag{4}$$

where $G(k,\omega) = \dfrac{1}{N_c}\sum\limits_{i,j}\text{e}^{\text{i}k(i-j)}G_{i,j}(k,\omega)$ is obtained from Eq.(3) by Fourier transforming over the cluster sites. The corresponding density of state (DOS) is obtained by summing over all wave vectors

$$N(\omega) = \sum_{k} A(k,\omega). \tag{5}$$

3. Results and discussion

In the present study, we use a cluster size of $N_c = 8$. The size dependence of the CPT spectral function is an important issue. Several investigations on this issue for the 1D Hubbard model[39−41] have concluded that the main features of the spectral function can be captured even for a modest cluster size $N_c = 8$. The parameter η has been set to be 0.1 in order to give δ peaks a finite width, and all energies are measured in units of t.

In figure 1 we present results for the single-particle spectral function $A(k,\omega)$ of the frustrated Hubbard model at half filling with specific parameters to examine the validity of the numerical method. For the case of $t' = 0$ ($t \neq 0$), the model is equivalent to the

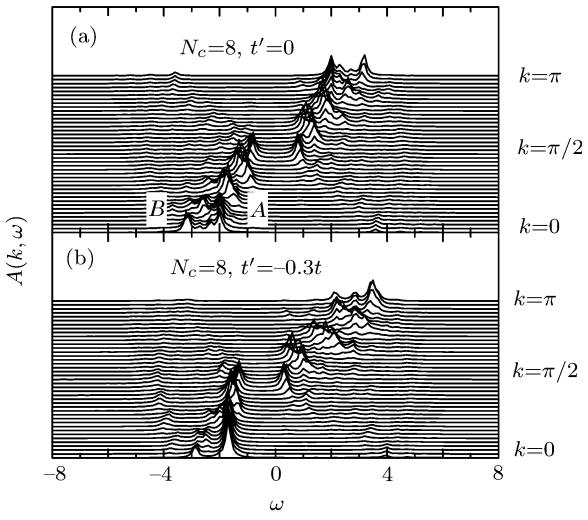


Fig.1. Spectral weight $A(k,\omega)$ at half filling for $U = 4t$ with different frustrations (a) $t' = 0$ and (b) $t' = -0.3t$ obtained by CPT for the cluster size $N_c = 8$.

ordinary 1D Hubbard model. Here, the occurrence of spin-charge separation with spinon A and holon B branches can be clearly identified, although one cannot really speak of a Luttinger liquid, since the system is an insulator. The spectral function displays a gap with a minimum at $k = \pi/2$.[41–44] The spectral weight below ($\omega \leq 0$) and above ($\omega \geq 0$) the Fermi energy corresponds to the photoemission (PES) and inverse photoemission spectrum (IPES), respectively.[45] As t' is turned on (figure 1(b)), the particle hole symmetry is destroyed ($A(k,\omega) \neq A(\pi - k, -\omega)$) as the lattice is frustrated by the next-nearest-neighbor hopping.

Figure 2 displays the single-particle spectral function $A(k,\omega)$ with different wave vectors k at half-filling for on-site interaction $U = 4t$. For smaller frustration hopping t' up to $0.5t$, the spectrum exhibits a Mott gap near the Fermi surface as shown in figure 2(a).

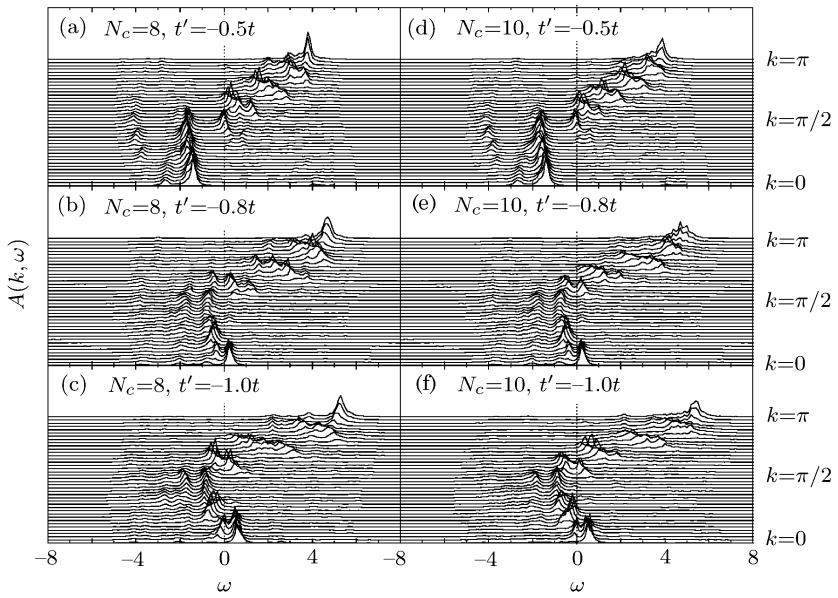


Fig.2. Single-particle spectral function $A(k,\omega)$ at half-filling for $U = 4t$ plotted as a function of energy ω for different momenta k. We present results for different values of t'. (a)–(c) the cluster size is $N_c = 8$; (d)–(f) the cluster size is $N_c = 10$.

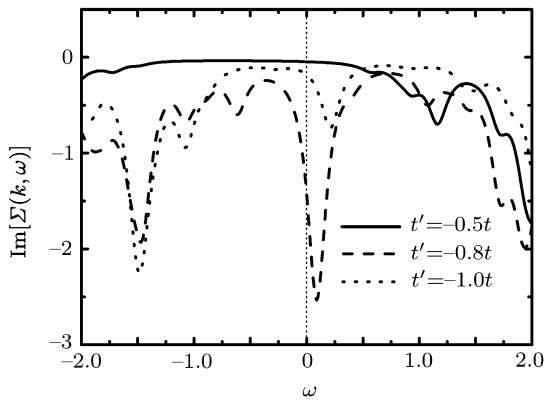


Fig.3. Imaginary part of the self-energy $\Sigma(k,\omega)$ for various frustration hoppings with $U = 4t$ at $k = \pi/8$ at half-filling.

When t' becomes larger, for instance $t' = -0.8t$, the gap evolves into a pseudogap (figure 2(b)). In order to check effects originating from the finite size of the cluster, we compare in figure 2 results for $N_c = 8$ and $N_c = 10$. As one can see from the figure, differences are negligible, which makes us confident that a cluster size $N_c = 8$ is sufficient for our calculation. To address the origin of the PG, we display in figure 3 the imaginary part of the self-energy, i.e. the scattering rate.[23,34,36] For $t' = -0.5t$, the imaginary part of the self-energy is very small around $\omega \sim 0$. When t' approaches $-0.8t$, the scattering rate becomes larger,

leading to the PG in the single-particle spectral. However, the scattering rate again decreases in magnitude for $t' = -1.0t$, leading to the disappearance of PG at large t'. Clearly, a large scattering rate leads to a removal of spectral weight which results in the appearance of PG.

Our results show that the frustration hopping t' is an important quantity in the present model, and plays an important role in the modulation of the spectral weight. In order to clarify the dependence of PG on the frustration t', we display the local DOS in figure 4. As pointed out in Ref.[24], an insulator-to-metal transition occurs with increasing t' for fixed U. However, by continuity, the overall gap structure is not expected to disappear discontinuously with increasing t'. Therefore, in the metallic state originating when t' exceeds a certain threshold, the insulating gap evolves into a pseudogap, characterised by two peaks around the Fermi level with a nonvanishing spectral weight between them. The gap scale (defined as the distance between peaks) and the gap depth decreases with further increase of the frustration hopping. This behavior is closely connected with the decrease of the imaginary part of self-energy shown in figure 3.

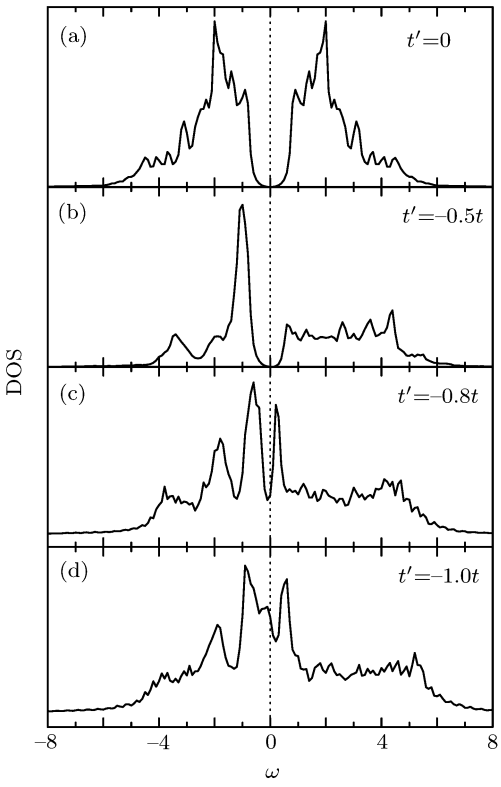


Fig.4. The density of state $N(\omega)$ with different t' for $U = 4t$.

In order to see how the frustration induced PG arises for different interaction strengths, we plot the DOS for several values of U in figure 5. The PG scale with fixed frustration hopping t' is found to be strongly dependent on the Hubbard interaction U. In the weak-coupling case, $N(\omega)$ only shows a small dip at the Fermi energy, indicating the existence of a PG structure. As U is increased beyond $5t$, the PG evolves into a gapped state. When U is further increased, the depth of the gap increases and a full Mott insulating gap develops. At the same time the position of the inner and Hubbard bands remain unchanged. Figure 5 displays a metal-insulator transition from a PG state at weak coupling ($U \leq 4t$) to a Mott–Hubbard insulator at a strong coupling ($U \geq 4t$). A PG is observed below the Mott transition.[46] The frustration-hopping-induced PG occurs only at relatively large values of t'/U.[47]

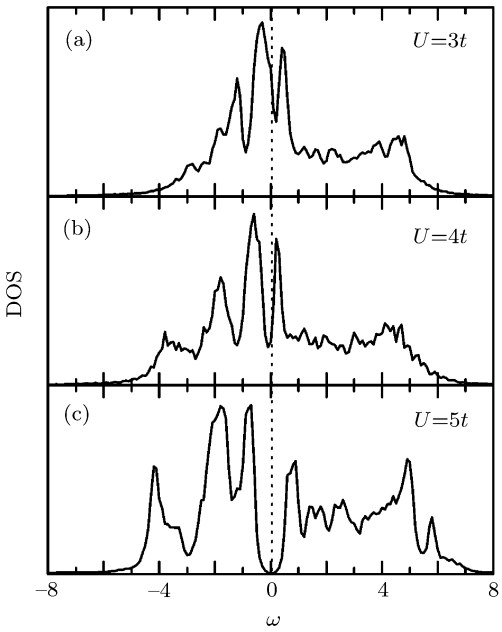


Fig.5. The density of state $N(\omega)$ for different values of U and $t' = -0.8t$.

Next we investigate the frustration induced PG at finite doping in the hole-doped system. The spectral function and DOS of a 12.5% hole-doped system with $t' = -0.5t$ and several values of U are shown in figure 6 and figure 7, respectively. The Mott gap does not appear to change as a function of doping but moves to the inverse photoemission side. On the other hand, the PG behaves quite differently, and it remains pinned around the Fermi energy upon hole doping. As shown in the figures, the dependence of the PG on U is much weaker at finite doping than at half filling,

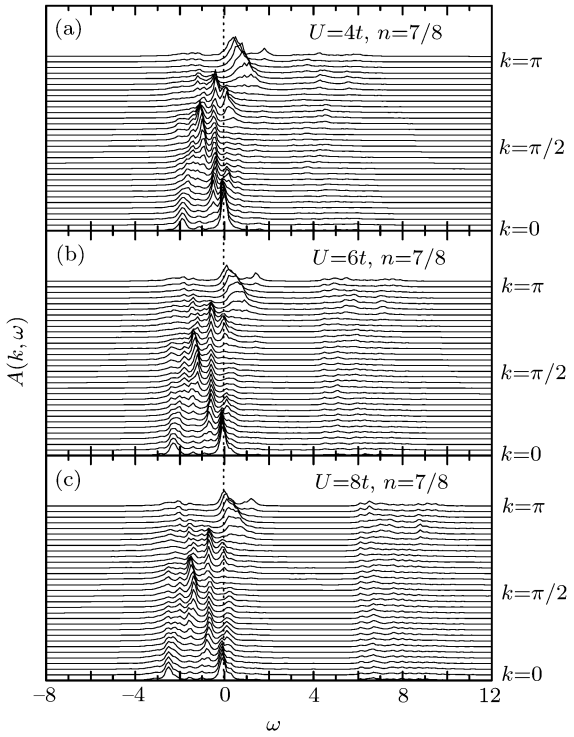


Fig.6. Single-particle spectral weight for 12.5% hole-doping. In all cases we use $t' = -0.5t$. The PG is pinned at the Fermi energy (dotted line) while the Mott gap is shifted in energy. The cluster size is $N_c = 8$.

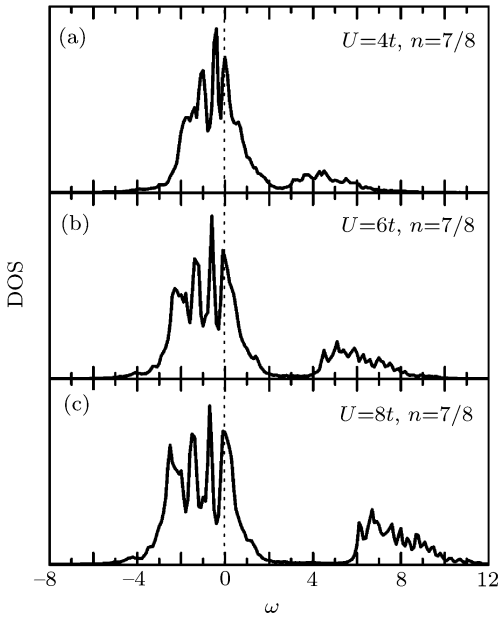


Fig.7. Density of states $N(\omega)$ for 12.5% hole-doping for various values of the Hubbard interaction U. All other parameters are the same as in figure 6.

and only a small change of the PG size is observed upon increasing U from $4t$ to $8t$. This suggests that hole doping favors the existence of PG. Therefore, we can deduce that the suppression of the PG with increasing U in the undoped system (figure 5) is dominantly caused by the increase of the Mott gap rather than the change of PG itself. Moreover, we notice that the spectral weight of the upper Hubbard band shifts into the lower-Hubbard band upon hole-doping.[48] This feature is attributed to the hole rich condition, as it is much easier for an added electron to occupy an empty state than to occupy an already occupied state with opposite spin since it needs larger energy.[45]

4. Summary

In summary, we have investigated the frustration induced PG in the frustrated Hubbard chain by computing the single-particle spectral function $A(k, \omega)$ and the DOS $N(\omega)$ at half-filling and at finite hole doping, within the CPT approximation. The next-nearest-neighbor hopping frustrates the system, breaks the particle-hole symmetry of the DOS, and produces a PG. The PG in the system originates in the transition between the gapful Mott insulator phase and the gapless conductor phase. In the undoped system, a full gap opens gradually with further increase of U and a PG is clearly observed only for a relatively large t'/U. At finite doping, the PG is no longer strongly dependent on U. Here, the PG and the Mott gap are separated in energy, and the Mott gap increases with increase of U.

References

[1] Damascelli A, Hussain Z, and Shen Z X 2003 *Rev. Mod. Phys.* **75** 473

[2] Wuyts B, Moshchalkov V V and Bruynseraede Y 1996 *Phys. Rev.* B **53** 9418

[3] Hinkov V, Bourges P, Pailhes S *et al* 2007 *Nature Phys.* **3** 780

[4] Takabatake T, Nakamoto G, Tanaka H, Fujii H, Nishigori S, Suzuki T, Fujita T, Ishikawa M, Oguro I, Kurisu M, and Menovsky A A 1993 *Transport and Thermal Properties of f-Electron Systems* (New York: Plenum) p111

[5] Emery V J and Kivelson S A 1995 *Nature* **347** 434

[6] Uemura Y J, Luke G M, Sternlieb B J, Brewer J H, Carolan J F, Hardy W N, Kadono R, Kempton J R, Kiefl R F, Kreitzman S R, Mulhern P, Riseman T M, Williams D L, Yang B X, Uchida S, Takagi H, Gopalakrishnan J, Sleight A W, Subramanian M A, Chien C L, Cieplak M Z, Xiao G, Lee V Y, Statt B W, Stronach C E, Kossler W J and Yu X H 1998 *Phys. Rev. Lett.* **62** 2317

[7] Lee P A and Wen X G 1997 *Phys. Rev. Lett.* **78** 4111

[8] Anderson P W 1987 *Science* **235** 1196
[9] Aichhorn M and Arrigoni E 2005 *Europhys. Lett.* **72** 117
[10] Liu X D, Xu X S, Wang Y Q, Zhang D Z and Cheng B Y 2003 *Chin. Phys.* **12** 992
[11] Warren W W, Walstedt R E, Brennert G F, Cava R J, Tycko R, Bell R F, and Dabbagh G 1989 *Phys. Rev. Lett.* **62** 1193
[12] Alloul H, Ohno T, and Mendels P 1989 *Phys. Rev. Lett.* **63** 1700
[13] Ronning F, Sasagawa T, Kohsaka Y, Shen K M, Damascelli A, Kim C, Yoshida T, Armitage N P, Lu D H, Feng D L, Miller L L, Takagi H and Shen Z X 2003 *Phys. Rev.* B **67** 165101
[14] Gruner G 2001 *J. Phys. Chem. Sol.* **62** 89
[15] Claessen R, Schwingenschlögl U, Sing M, Jacobosen C S and Dressel M 2002 *Physica* B **312** 660
[16] Mourachkine A 2001 *Supercond. Sci. Technol.* **14** 329
[17] Valbuena M A, Avila J, Pantin V, Drouard S, Guyot H and Asensio M C 2006 *Appl. Sur. Sci.* **252** 5415
[18] Zwick F, Jérome D, Margaritondo G, Onellion M, Voit J and Grioni M 1998 *Phys. Rev. Lett.* **81** 2974
[19] Medicherla V R R, Patil S, Singh R S and Maiti K 2007 *Appl. Phys. Lett.* **90** 062507
[20] Pimenov A V, Boris A V, Yu L, Hinkov V, Wolf T, Tallon J L, Keimer B and Bernhard C 2005 *Phys. Rev. Lett.* **94** 227003
[21] Kim C, Matsuura A Y, Shen Z X, Motoyama N, Eisaki H, Uchida S, Tohyama T and Maekawa S 1996 *Phys. Rev. Lett.* **77** 4054
[22] Valentí R, Saha-Dasgupta T, Alvarez J V, Požgajčić K and Gros C 2001 *Phys. Rev. Lett.* **86** 5381
[23] Stanescu T D and Phillips P 2003 *Phys. Rev. Lett.* **91** 017002
[24] Daul S and Noack R M 2000 *Phys. Rev.* B **61** 1646
[25] Hamacher K, Gros C and Wenzel W 2002 *Phys. Rev. Lett.* **88** 217203
[26] Japaridze G I, Noack R M and Baeriswyl D 2006 cond-mat/0607054
[27] Pandey S and Singh A 2007 *Phys. Rev.* B **75** 064412
[28] Torio M E , Aligia A A and Ceccatto H A 2003 *Phys. Rev.* B **67** 165102
[29] Huang Z B, Hanke W, Arrigoni E and Chubukov A V 2006 *Phys. Rev.* B **74** 184508
[30] Civelli M, Capone M, Kancharla S S, Parcollet O and Kotliar G 2005 *Phys. Rev. Lett.* **95** 106402
[31] Bartosch L 2003 *Phys. Rev. Lett.* **90** 076404
[32] Arrigoni E and Aichhorn M 2006 *Physica* B **378**, 432
Aichhorn M, Arrigoni E, Potthoff M and Hanke W 2006 *Phys. Rev.* B **74** 024508
[33] Macridin A, Jarrell M, Maier T, Kent P R C and D'Azevedo E 2006 *Phys. Rev. Lett.* **97** 036401
[34] Kyung B, Kancharla S S, Sénéchal D, Tremblay A M S, Civelli M and Kotliar G 2006 *Phys. Rev.* B **73** 165114
[35] Arrigoni E 1999 *Phys. Rev. Lett.* **83** 128
Arrigoni E 1998 *Phys. Rev. Lett.* **80** 790
Zacher M G, Eder R, Arrigoni E and Hanke W 2000 *Phys. Rev. Lett.* **85** 2585
Zacher M G, Eder R, Arrigoni E and Hanke W 2002 *Phys. Rev.* B **65** 045109
[36] Sénéchal E and Tremblay A M S 2004 *Phys. Rev. Lett.* **92** 126401
[37] Gros C and Valenti R 1993 *Phys. Rev.* B **48** 418
Ovchinnikov S G and Sandalov I S 1989 *Physica* C **161** 607
[38] Dagotto E 1994 *Rev. Mod. Phys.* **66** 763
[39] Sénéchal D, Perez D and Pioro-Ladriére M 2000 *Phys. Rev. Lett.* **84** 522
[40] Zhao H, Wu C Q and Lin H Q 2005 *Phys. Rev.* B **71** 115201
[41] Ning W Q, Zhao H, Wu C Q and Lin H Q 2006 *Phys. Rev. Lett.* **96** 156402
[42] Zacher M G, Arrigoni E, Hanke W and Schrieffer J R 1998 *Phys. Rev.* B **57** 6370
[43] Benthien H, Gebhard F and Jeckelmann E 2004 *Phys. Rev. Lett.* **92** 256401
[44] Matsueda H, Bulut N, Tohyama T and Maekawa S 2005 *Phys. Rev.* B **72** 075136
[45] Wang W Z, Hu B and Yao K L 2002 *Phys. Rev.* B **66** 085101
[46] Zhang Y Z and Imada M 2007 *Phys. Rev.* B **76** 045108
[47] Refolio M C, L'opez Sancho J M and Rubio J 2002 *Phys. Rev.* B **65** 075114
[48] Eskes H, Meinders M B J and Sawatzky G A 1991 *Phys. Rev. Lett.* **67** 1035