Suppression of *d*-wave superconductivity in the checkerboard Hubbard model

D. G. S. P. Doluweera,[1,3] A. Macridin,[1] T. A. Maier,[2] M. Jarrell,[1] and Th. Pruschke[3]

[1]*University of Cincinnati, Cincinnati, Ohio 45221, USA*
[2]*Oak Ridge National Laboratory, Oak Ridge, Tennessee 37831, USA*
[3]*Institut für Theoretische Physik, Universität Göttingen, Friedrich-Hund-Platz 1, 37077 Göttingen, Germany*

Using a dynamical cluster quantum Monte Carlo approximation, we investigate the *d*-wave superconducting transition temperature T_c in the doped two-dimensional repulsive Hubbard model with a weak inhomogeneity. The inhomogeneity is introduced in the hoppings t' and t in the form of a checkerboard pattern where t is the hopping within a 2×2 plaquette, and t' is the hopping between the plaquettes. We find inhomogeneity suppresses T_c. The characteristic spin excitation energy and the strength of *d*-wave pairing interaction decrease with decreasing T_c, suggesting a strong correlation between these quantities.

I. INTRODUCTION

The role of inhomogeneity in high temperature superconductors (HTS) is still an unsettled issue. Neutron scattering experiments reveal the presence of one-dimensional (1D) charge and spin microscopic inhomogeneities (stripes) in underdoped HTS (Refs. 1–4) above the superconducting transition temperature T_c. Scanning tunneling microscopic imaging provides evidence for the presence of two-dimensional (2D) real-space or local-density-of-states modulations called checkerboard patterns in Bi-2212 (Refs. 5–8) and Na-CCOC (Refs. 9 and 10) superconducting samples. Inhomogeneities observed in cuprates led to theoretical scenarios for an inhomogeneity based pairing mechanism in HTS.[11,12] Other theoretical studies[13–16] argue that inhomogeneities can enhance pairing and T_c.

The checkerboard model[16] we investigate is sketched in the upper panel of Fig. 1. It is homogeneous when $t'=t$ and inhomogeneous when $t' \neq t$. Here t (t') is the hopping amplitude within (between) the cluster(s). The low-temperature phase diagram of the checkerboard Hubbard model (CBHM) in the strongly inhomogeneous limit ($t' \ll t$), i.e., with weakly coupled clusters, was studied in Refs. 16 and 17. For small $t' \ll t$ and for values of on-site interaction $U \approx 4.58t$, the authors find a *d*-wave superconducting state in addition to a variety of other phases. Their results led them to expect a maximum of T_c at an optimal $t' < t$. Other authors[18,19] found a *d*-wave superconducting state with a significant T_c for the homogeneous case ($t'=t$) in the 2D Hubbard model. Therefore, it is interesting to see if the inhomogeneous CBHM has a higher T_c compared to the homogeneous model. This is especially important in the weak inhomogeneity regime not addressed before since experimentally observed inhomogeneities in the cuprates are weak.

In this paper we investigate *d*-wave superconductivity in the CBHM near the homogeneous limit, i.e., for a weakly inhomogeneous system. We use the dynamical cluster approximation (DCA) (Ref. 20) to calculate T_c as a function of t'. DCA is a momentum (k) space formulation suitable to study the problem since our interest is around the homogeneous limit. We find that a weak inhomogeneity suppresses T_c. At fixed values of U/W and U/t with doping δ appropriate for HTS, T_c decreases for $t' \neq t$. Therefore, we find a maximum T_c in the homogeneous system. Furthermore, cal-

culations with fixed U/t for $t' < t$ show that T_c decreases proportionally to the characteristic spin excitation energy and the strength of the *d*-wave pairing interaction, suggesting a strong correlation between them.

II. FORMALISM

The DCA maps the lattice problem onto a periodic cluster embedded in a self-consistent host. Short-range correlations up to the linear cluster size L_c are treated explicitly while longer-range correlations are treated in a dynamical mean-field manner. We use a quantum Monte Carlo (QMC) method to solve the cluster problem. We use the maximum entropy method to analytically continue imaginary time QMC data to real frequencies.[21]

The Hamiltonian of our model is

$$H = - \sum_{\langle ij \rangle \sigma} t_{ij}(c_{i\sigma}^{\dagger} c_{j\sigma} + c_{j\sigma}^{\dagger} c_{i\sigma}) + U \sum_{i} n_{i\sigma} n_{i-\sigma}, \quad (1)$$

where $c_{i\sigma}^{\dagger}$ ($c_{i\sigma}$) creates (destroys) an electron at site i with spin σ and $n_{i\sigma}=c_{i\sigma}^{\dagger} c_{i\sigma}$. Here $\langle ij \rangle$ denotes the nearest-neighbor sites i and j. As shown in Fig. 1, $t_{ij}=t(t_{ij}=t')$, when i and j belong to the same (neighboring) plaquette(s). U is the local Coulomb repulsion and it is site independent.

Here we present results obtained for a $N_c=4$ site cluster (2×2 sites). $N_c=4$ is the smallest cluster that contains one *d*-wave plaquette and allows for a *d*-wave superconducting state.[18] It has been intensively studied in the last few years.[22] It has the advantage that the QMC sign problem is mild, thus allowing the investigation of physics at low temperatures. However, since it contains only one *d*-wave plaquette, it does not capture *d*-wave phase fluctuations and hence overesti-
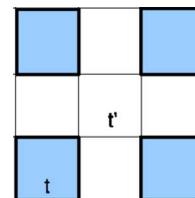

FIG. 1. (Color online) 2×2 plaquette model. Here t is intracluster hopping and t' is intercluster hopping.
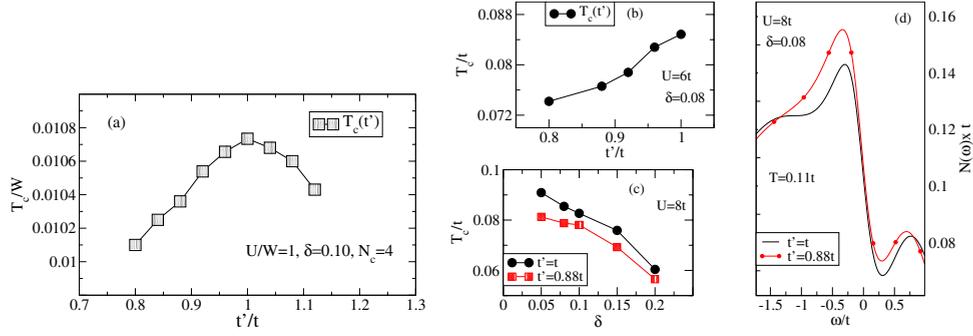
FIG. 2. (Color online) (a) $T_c(t')/W$ for $U/W=1$ and at 10% doping. T_c is suppressed for $t' \neq t$. (b) $T_c(t')/t$ for $U=6t$ and at 8% doping. T_c monotonically decreases with decreasing t'. (c) T_c/t for $t'=t$ and $t'=0.88t$ as a function of doping δ when $U=8t$. (d) Low-energy density of states $N(\omega)t$ for $t'=t$, and $t'=0.88t$ at $T=0.11t$ for 8% doping and $U=8t$. Note the increase in low-energy spectral weight for $t'=0.88t$.

mates T_c.[18] Calculations for larger clusters that capture these fluctuations will be an interesting future work. Details of the full DCA formalism applied to the CBHM will be published elsewhere.[23]

T_c and the Néel temperature (T_N) are the temperatures where the superconducting and antiferromagnetic suscepti-bilities diverge. For small clusters it may be approximately described as the temperature at which the superconducting correlation length exceeds the linear cluster size. In a mean-field calculation such as DCA, the transition temperature is overestimated and decreases with increasing cluster size.[22] As we are treating the model in an elaborate mean-field scheme, the phase transition signaled by the divergence will quite likely not be present in the real 2D system but may survive as a Kosterlitz-Thouless transition, at least for d-wave superconductivity.[18]

T_c can be obtained from the temperature dependence of the pairing matrix $M(K,K')=\Gamma^{pp}(K,K')\chi^0(K',K)$. Here, $K=(\mathbf{K},i\omega_n)$, $\Gamma^{pp}(K,K')$ (pairing interaction) is the irreducible particle-particle vertex and the bare bubble, $\chi^0(K',K)$, is the coarse-grained product of two fully dressed single-particle Green's functions, $G(k,k')$ and $G(-k,-k')$. $\omega_n=(2n+1)\pi T$ is the Matsubara frequency at temperature T. We determine T_c from the temperature dependence of the leading eigen-value $\lambda(T)$ of M.[24,25] We find T_c from $\lambda(T_c)=1$ and the sym-metry of the superconducting state is determined by the sym-metry of the corresponding eigenvector, $\Phi(K)$, of M. For the investigated range of t', we find that the leading eigenvector $\Phi_d(K)$ has d-wave symmetry.

We define the strength of the pairing interaction, V_d, by projecting out the pairing vertex, Γ^{pp}, to the d-wave sub-space, as

$$V_d(T) = \frac{1}{N_c}\sum_{\mathbf{K}\mathbf{K}'} g(\mathbf{K})\Gamma^{pp}(\mathbf{K},\pi T;\mathbf{K}',\pi T)g(\mathbf{K}'). \quad (2)$$

Here $g(\mathbf{K})=\cos(\mathbf{K}_x)-\cos(\mathbf{K}_y)$ is the d-wave form factor. Correspondingly, we define the d-wave projected bare bubble as

$$P_{d0}(T) = \frac{1}{N_c}\sum_{\mathbf{K}\mathbf{K}'} g(\mathbf{K})\chi^0_{pp}(\mathbf{K},\mathbf{K}',\pi T)g(\mathbf{K}'). \quad (3)$$

V_d and P_{d0} were initially introduced in Ref. 28. They satisfy the approximation $V_d(T)P_{d0}(T) \approx \lambda_d(T)$.

III. RESULTS

Since the bandwidth $W=4(t+t')$ of the inhomogeneous system changes with t', we could use either W or the maxi-mum of t and t' as a unit of energy. Since both the Hamil-tonian and W are symmetric under the interchange of t and t', in both cases the results should reflect this symmetry. The first choice compensates for changes in T_c due to changes of the kinetic energy. The second choice reflects the hopping suppression due to inhomogeneity and will produce perfectly symmetric plots with abscissa t'/t around one.

We find that both of these choices lead to the same main conclusion that the inhomogeneity suppresses T_c. In Fig. 2(a) we show results when W is taken as the energy unit for $U/W=1$ and at 10% doping. T_c is maximum in the homoge-neous limit $t'/t=1$. In the subsequent figures throughout the paper, we will present results for the case where the energy unit is given by t. As can be seen from Fig. 2(b), where the $U=6t$ at 8% doping case is shown, T_c monotonically de-creases with decreasing t'. The suppression of T_c due to in-homogeneity occurs on the doping range appropriate for HTS. This can be seen in Fig. 2(c), where we show T_c vs δ (Ref. 27) for $U=8t$. Note that the inhomogeneous system with $t'=0.88t$ has a lower T_c than the homogeneous system on the doping range 2–20%.

We find that $t' \leq t$ enhances the density of states $N(\omega)$ at low excitation energy ($-0.5t < \omega < 0.5t$). This can be seen in Fig. 2(d) where $N(\omega)$ for $t'=0.88t$ and $t'=t$ are compared at 8% doping for $U=8t$. The enhancement of $N(\omega)$ is a band-structure effect since it can also be noticed for the noninter-acting problem, i.e., when $U=0$. The low-energy part of $N(\omega)$ has an important role in determining the value of T_c.

We find two competing effects of t' on the pairing matrix as captured by V_d and P_{d0}. Figure 3(a) shows the t' depen-dence of V_d, P_{d0}, and T_c for $U=6t$ at 8% doping. $V_d(t')$ and $P_{d0}(t')$ are shown at a temperature equal to the homogeneous T_c, i.e., $T_{c\text{-hom}}$, and are normalized to their values at $t'=t$ for easy comparison. V_d decreases with decreasing t', indicating a decreasing d-wave contribution to Γ^{pp} as t' decreases. The effect of t' on χ^0 is captured by P_{d0}. $P_{d0}(t')$ increases with decreasing t'. Since P_{d0} is related to $N(\omega)$ through G, this behavior is related to the enhanced low-energy part of $N(\omega)$ discussed previously. The effects of t' on V_d and P_{d0} provide a qualitative description of the behavior of T_c since $V_d(T)P_{d0}(T) \approx \lambda_d(T)$. Note that the relative decrease in V_d is
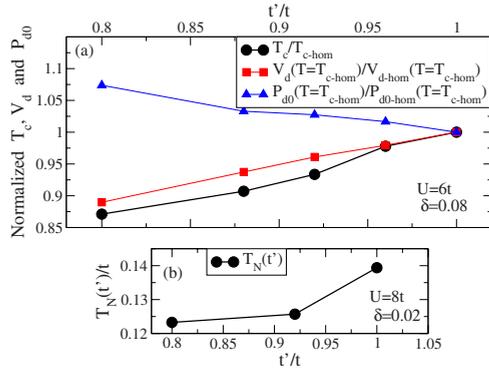
FIG. 3. (Color online) (a) Normalized values of T_c, V_d, and P_{d0} as a function of t' at 8% doping, $U=6t$, and $N_c=4$. V_d and P_{d0} are described in the text. (b) Néel temperature T_N/t for different values of t' at 2% doping for $U=8t$.

FIG. 4. (Color online) (a) Magnetic structure factor $S(Q,\omega)$ for $U=6t$, $\delta=0.08$, and temperature $T=0.087t$ at $Q=(0,\pi)$ for different values of t'. The location of the peak is a measure of the characteristic spin excitation energy, here defined as J_{eff}. The inset of (a) is blown up to show the area around peak positions. $T_c(t')$ and $J_{\mathrm{eff}}(t',T=0.087t)$ are normalized to their values at $t'=t$, as a function of t' for (b) $U=6t$ and $\delta=0.08$, (c) $U=8t$ and $\delta=0.08$, and (d) $U=8t$ and $\delta=0.15$. Note that both normalized $T_c(t')$ and $J_{\mathrm{eff}}(t')$ monotonically increase with t'.

always larger than the relative increase in P_{d0}. Therefore, the net effect of t' is to reduce T_c. The behavior of $V_d(t')$ and $P_{d0}(t')$ at other values of U and δ (not shown) is similar, leading to a suppression of superconductivity.

Using the DCA for the homogeneous 2D Hubbard model, it was previously shown that the dominant part of the pairing interaction comes from the $S=1$ particle-hole magnetic channel.[25] The energy scale of spin excitations is characterized by the superexchange interaction, $J=4t^2/U$, and changing the hopping matrix elements of the homogeneous problem will also influence J. However, the relationship between T_c and the characteristic energy scale of spin excitations in the weakly inhomogeneous system is not known. Therefore it is worth studying the effect of t' on the Néel temperature and on the spin excitations as characterized by the magnetic structure factor $S(\mathbf{Q},\omega)$.

We find that at small doping, T_N decreases with decreasing t', as shown for $U=8t$ at 2% hole doping in Fig. 3(b). As discussed before for a finite-size cluster, T_N occurs when the antiferromagnetic correlation length ζ_{AF} exceeds the linear cluster size. Therefore, decreasing ζ_{AF} indicates the suppression of antiferromagnetism in the weakly inhomogeneous system for small δ compared to a homogeneous system.

The magnetic structure factor $S[\mathbf{Q}=(0,\pi),\omega]$ for various t' values is shown in Fig. 4(a) for $U=6t$ at 8% doping. The location of the peak of $S[\mathbf{Q}=(0,\pi),\omega]$ can be considered a measure of the characteristic spin excitation energy and we define its position to be $2J_{\mathrm{eff}}$. This is done in analogy with linear spin-wave theory[29–31] where the peak of the structure factor at $\mathbf{Q}=(0,\pi)$ is at energy $2J$, J being the superexchange nearest-neighbor spin interaction. Note that $J_{\mathrm{eff}}(t')$ decreases with decreasing t', showing that a weak inhomogeneity softens the high energy spin excitations. This can be seen from the plot of $S[\mathbf{Q}=(0,\pi),\omega]$ in Fig. 4(a) and plots of $J_{\mathrm{eff}}(t')$ in Figs. 4(b)–4(d).

We find that $T_c \propto J_{\mathrm{eff}}$, as suggested from Figs. 4(b)–4(d). By comparing 8% doping [Figs. 4(b) and 4(c)] with 15% doping [Fig. 4(d)], one can see that this proportionality holds better for small doping. The proportionality between T_c and the superexchange interaction J are in accordance with the experimental observations reported in Ref. 32, and the computational investigation on the homogeneous system in Ref. 19.
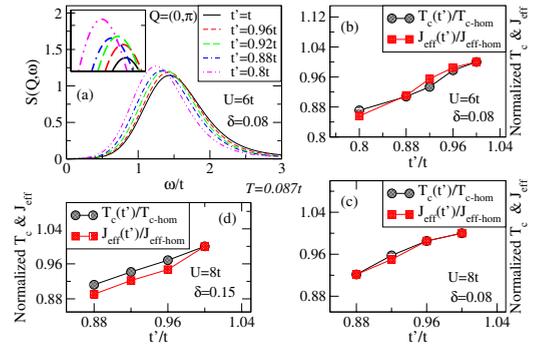
IV. DISCUSSION

The maximum T_c occurs in the homogeneous system and it is suppressed by weak inhomogeneity. The suppression of T_c prevails over the investigated range of doping δ and U, which are appropriate for a description of HTS. A recent experiment on Na doped $Ca_2CuO_2Cl_2$ (Na-CCOC) also indicates suppression of T_c due to inhomogeneity over a wide range of doping.[10]

According to our analysis, the suppression of T_c due to weak inhomogeneity is accompanied by a suppression of V_d and J_{eff}. This is an important observation since it suggests a strong correlation between the characteristic spin excitation energy J_{eff} and the pairing interaction. It is consistent with the previous finding that the pairing interaction in the 2D Hubbard model is dominated by the $S=1$ magnetic channel[25] and other results reported by Maier et al.[28,33] Therefore inhomogeneities that reduce magnetic contributions to the pairing interaction are likely to reduce d-wave superconductivity.

Since we find $T_c \propto J_{\mathrm{eff}}$, it may be possible to increase T_c by enhancing J_{eff}. In our model we find that a weak inhomogeneity decreases J_{eff} but other kinds of inhomogeneity might increase J_{eff} and, thus, if our assumption is correct, enhance T_c. For example, weak on-site disorder seems to increase J in the vicinity of defects.[34]

Regarding the speculation for the existence of an optimal inhomogeneity raised in Ref. 16, our results based on the $N_c=4$ cluster indicate that T_c is an increasing function of t' in the weakly inhomogeneous system and the optimal t' occurs at $t'=t$. Therefore our results for the weakly inhomogeneous system are not in agreement with this speculation but they do not exclude the possibility for an optimal t' at smaller values of t'. In addition, it will also be interesting to see how T_c scales with cluster size N_c when the weak inhomogeneity is present.

V. CONCLUSION

Using the dynamical cluster approximation for a $N_c=4$ cluster, we find that a weak inhomogeneity in the checker-

board Hubbard model suppresses *d*-wave superconductivity. The characteristic spin excitation energy and the strength of the pairing interaction decrease along with decreasing T_c, suggesting a strong correlation between these quantities.

Note added in proof. After the manuscript was accepted for publication we learned about exact diagonalization results for the checkerboard model on small Hubbard clusters.[35]

ACKNOWLEDGMENTS

[1] J. M. Tranquada, B. J. Sternlieb, J. D. Axe, Y. Nakamura, and S. Uchida, Nature (London) **375**, 561 (1995).

[2] H. A. Mook, Pengcheng Dai, F. Dogan, and R. D. Hunt, Nature (London) **404**, 729 (2000).

[3] R. P. Sharma, S. B. Ogale, Z. H. Zhang, J. R. Liu, W. K. Chu, Boyed Veal, A. Paulikas, H. Zheng, and T. Venkatesan, Nature (London) **404**, 736 (2000).

[4] V. Hinkov, S. Pailhs, P. Bourges, Y. Sidis, A. Ivanov, A. Kulakov, C. T. Lin, D. P. Chen, C. Bernhard, and B. Keimer, Nature (London) **430**, 650 (2004).

[5] C. Howald, H. Eisaki, N. Kaneko, M. Greven, and A. Kapitulnik, Phys. Rev. B, **67**, 014533 (2003); C. Howald, H. Eisaki, N. Kaneko, and A. Kapitulnik, Proc. Natl. Acad. Sci. U.S.A. **100**, 9705 (2003).

[6] J. E. Hoffman, E. W. Hudson, K. M. Lang, V. Madhavan, H. Eisaki, S. Uchida, and J. C. Davis, Science **295**, 466 (2002).

[7] M. Vershinin, S. Misra, S. Ono, Y. Abe, Y. Ando, and A. Yazdani, Science **303**, 1995 (2004).

[8] K. McElroy, D.-H. Lee, J. E. Hoffman, K. M. Lang, J. Lee, E. W. Hudson, H. Eisaki, S. Uchida, and J. C. Davis, Phys. Rev. Lett. **94**, 197005 (2005).

[9] T. Hanaguri, C. Lupien, Y. Kohsaka, D.-H. Lee, M. Azuma, M. Takano, H. Takagi, and J. C. Davis, Nature (London) **430**, 1001 (2004).

[10] D. Hirai, T. Sasagawa, and H. Takagi, Physica C **463–465**, 56 (2007).

[11] E. W. Carlson, V. J. Emery, S. A. Kivelson, and D. Orgad, *The Physics of Superconductors*, edited by K. H. Bennemann and J. B. Ketterson (Springer-Verlag, New York, 2004), Vol. II, p. 275.

[12] E. Arrigoni, E. Fradkin, and S. A. Kivelson, Phys. Rev. B **69**, 214519 (2004).

[13] Ivar Martin, Daniel Podolsky, and Steven A. Kivelson, Phys. Rev. B **72**, 060502(R) (2005).

[14] K. Aryanpour, E. R. Dagotto, M. Mayr, T. Paiva, W. E. Pickett, and R. T. Scalettar, Phys. Rev. B **73**, 104518 (2006).

[15] Y. L. Loh and E. W. Carlson, Phys. Rev. B **75**, 132506 (2007).

[16] Wei-Feng Tsai and Steven A. Kivelson, Phys. Rev. B **73**, 214510 (2006); **76**, 139902(E) (2007).

[17] Hong Yao, Wei-Feng Tsai, and Steven A. Kivelson, Phys. Rev. B **76**, 161104(R) (2007).

[18] T. A. Maier, M. Jarrell, T. C. Schulthess, P. R. C. Kent, and J. B. White, Phys. Rev. Lett. **95**, 237001 (2005).

[19] Kristjan Haule and Gabriel Kotliar, Phys. Rev. B **76**, 104509 (2007).

[20] M. H. Hettler, A. N. Tahvildar-Zadeh, M. Jarrell, T. Pruschke, and H. R. Krishnamurthy Phys. Rev. B **58**, R7475 (1998); M. H. Hettler, M. Mukherjee, M. Jarrell, and H. R. Krishnamurthy, *ibid.* **61**, 12739 (2000).

[21] M. Jarrell and J. E. Gubernatis, Phys. Rep. **269**, 133 (1996).

[22] Th. Maier, M. Jarrell, Th. Pruschke, and M. Hettler, Rev. Mod. Phys. **77**, 1027 (2005).

[23] (unpublished).

[24] N. Bulut, D. J. Scalapino, and S. R. White, Phys. Rev. B **47**, 6157(R) (1993).

[25] T. A. Maier, M. S. Jarrell, and D. J. Scalapino, Phys. Rev. Lett. **96**, 047005 (2006).

[26] M. Jarrell, Th. Maier, M. H. Hettler, and A. N. Tahvildarzadeh, Europhys. Lett. **56**, 563 (2001).

[27] The T_c vs δ phase diagram of the homogeneous system found with the $N_c = 4$ cluster has been discussed in Ref. [26].

[28] T. A. Maier, M. Jarrell, and D. J. Scalapino, Phys. Rev. B **74**, 094513 (2006).

[29] It is reasonable to view HTS as doped antiferromagnetic Mott-insulators (Ref. [30]) and magnetic excitations may be approximated by the magnon dispersion given by linear spin-wave theory. These magnon excitations show a peak at $\mathbf{Q} = (0, \pi)$ at an energy $\omega = 2J$ (Ref. [31]).

[30] Patrick A. Lee, Naoto Nagaosa, and Xiao-Gang Wen, Rev. Mod. Phys. **78**, 17 (2006).

[31] E. Manousakis, Rev. Mod. Phys. **63**, 1 (1991).

[32] Rinat Ofer, Galina Bazalitsky, Amit Kanigel, Amit Keren, Assa Auerbach, James S. Lord, and Alex Amato, Phys. Rev. B **74**, 220508(R) (2006).

[33] T. A. Maier, M. Jarrell, and D. J. Scalapino, Phys. Rev. B **75**, 134519 (2007); T. A. Maier, A. Macridin, M. Jarrell, and D. J. Scalapino, *ibid.* **76**, 144516 (2007).

[34] Maciej M. Maśka, Żaneta Śledź, Katarzyna Czajka, and Marcin Mierzejewski, Phys. Rev. Lett. **99**, 147006 (2007).

[35] W.-F. Tsai, H. Yao, A. Lauchli, and S. A. Kivelson, Phys. Rev. B **77**, 214502 (2008).