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Evidence for d-wave superconductivity in the repulsive Hubbard model

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Abstract. We perform numerical simulations of the Hubbard model using the projector Quantum Monte Carlo method. A novel approach for finite size scaling is discussed. We obtain evidence in favor of d-wave superconductivity in the repulsive Hubbard model. For $U = 4$, T_c is roughly estimated as $T_c \approx 30$ K.

PACS. 74.20.-z Theories and models of superconducting state – 71.10.Fd Lattice fermion models (Hubbard model, etc.) – 02.70.Lq Monte-Carlo and statistical methods

After the discovery of high-temperature superconductivity (HTSC) the two-dimensional Hubbard model (HM) [1,2] has been proposed as a model for a theoretical explanation of the phenomena. Indeed it has been shown, that the HM exhibits similar properties as the HTSC like a linear resistivity with the temperature [3] or the antiferromagnetism at half filling [4].

It is now widely accepted, that HTSC show d-wave symmetry of the superconducting order parameter [5,6]. According to [7,8], our simulations [9,10] and recent work [11,12] (for unisotrope hopping) the repulsive HM also favors d-wave symmetry. But the question of (d-wave) superconductivity in the repulsive HM has been discussed controversially [9–11].

We proposed the tt'-Hubbard model (tt'-HM) as the suited model for numerical simulations [9,10]. It exhibits a Van Hove singularity away from half filling [10]. Furthermore with the tuning of the next nearest neighbor hopping t' we are in the position to circumvent some of numerical difficulties in the simulation [13,14] by tuning the position of the finite size shells of the kinetic part of the HM. The tt'-HM is described by the Hamiltonian

$$\mathcal{H} = -t \sum_{\langle i,j\rangle,\sigma} c^{\dagger}_{i,\sigma} c_{j,\sigma} - t' \sum_{\langle\langle i,j\rangle\rangle,\sigma} c^{\dagger}_{i,\sigma} c_{j,\sigma} + U \sum_{i} n_{i,\uparrow} n_{i,\downarrow}. \tag{1}$$

Here $c^{\dagger}_{i,\sigma}$ creates an electron with spin σ on site i, $n_{i,\sigma}$ is the corresponding number operator and U is the on-site Coulomb interaction. The sum $\langle i,j\rangle$ ($\langle\langle i,j\rangle\rangle$) runs over the pairs of (next) nearest neighbors.

Our simulations are performed with the projector quantum Monte-Carlo method (PQMC) [15–17], in which the ground state

$$|\Psi_0\rangle = \frac{1}{\mathcal{N}} \mathrm{e}^{-\theta\mathcal{H}} |\Psi_{\mathrm{T}}\rangle \tag{2}$$

of the Hamiltonian $\mathcal{H}$ is projected from a testfunction $|\Psi_{\mathrm{T}}\rangle$ with a normalization constant $\mathcal{N}$ and with the projection parameter θ. Details of the method are described in [13].

To provide evidence for superconductivity we follow the standard concept of off diagonal long range order (ODLRO) [18]. According to [19] we study not the eigen values of the reduced two-particle density matrix, but only the equal times two-particle correlation function (CF)

$$C_{\mathrm{d}}(r) = \frac{1}{L} \sum_{i,\delta,\delta'} g_{\delta} g_{\delta'} \langle c^{\dagger}_{i\uparrow} c^{\dagger}_{i+\delta\downarrow} c_{i+r+\delta'\downarrow} c_{i+r\uparrow}\rangle \tag{3}$$

with the phase factors g_{δ}, $g'_{\delta} = \pm 1$ to model the d-wave symmetry, the number of lattice points L and the sum δ (δ') over all nearest neighbors. As first used in [20] we concentrate on the vertex CF

$$C^{\mathrm{V}}_{\mathrm{d}}(r) = C_{\mathrm{d}}(r) - \frac{1}{L} \sum_{i} \sum_{\delta,\delta'} g_{\delta} g_{\delta'} C^{\mathrm{one}}_{\uparrow}(i,r) \times C^{\mathrm{one}}_{\downarrow}(i+\delta, i+r+\delta') \tag{4}$$

with the single-particle CF $C^{\mathrm{one}}_{\sigma} \equiv \langle c^{\dagger}_{i,\sigma} c_{i+r,\sigma}\rangle$ for spin σ to extract the pairing effects in the two-particle CF. At this point we should note the simulations must be carried out in the right parameter regime. Especially for large U and L (as $U \geq 4$ and $L > 8 \times 8$) the fluctuations are so dramatic that no conclusions can be drawn from the vertex CFs of the simulations [13,21]. As shown in [9] and in further detail in [10] the d-wave correlations are positive for larger distances $|r|$ and level off to a "plateau". These results have been recently supported by [11]. Other

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Table 1. Lattice sizes $L = L_x L_x$ and number of electrons n_σ used in numerical simulations for $t' = -0.22$. (16×16 and $t' = 0$: $n_\sigma = 109$, $\langle n \rangle = 0.85$).

L	6×6	8×8	10×10	12×12	16×16
$n_\uparrow = n_\downarrow$	13	25	41	61	105
$\langle n \rangle$	0.72	0.78	0.82	0.85	0.82

superconducting symmetries (in particular s-wave) fluctuate around zero [22]. Our current simulations reach the same conclusion for the pure HM ($t' = 0$).

The question of superconductivity can be only answered by finite size scaling. In the case of weak or intermediate interaction [23] the behavior of the CF is dominated by the shell structure of the system. Considering the averaged vertex CF

$$\bar{C}_{\mathrm{d}}^{\mathrm{V}} \equiv \frac{1}{L} \sum_{r} C_{\mathrm{d}}^{\mathrm{V}}(r) \tag{5}$$

with the number $L = L_x^2$ of lattice points the standard $1/L_x$ scaling for instance seems to provide clear evidence against superconductivity [24,25] or the vanishing long range part of $C_{\mathrm{d}}(r)$ [11]. In this paper we argue that this conclusion is too simplified.

In this context we introduce a BCS-reduced model [26], the J-model, with the same kinetic Hamiltonian as the tt'-HM and a mean field interaction favoring cooper pairs with d-wave (s-wave) symmetry. In momentum space this model is described by the Hamiltonian

$$\mathcal{H} = \sum_{k,\sigma} \varepsilon_k c_{k,\sigma}^\dagger c_{k,\sigma} + \frac{J}{L} \sum_{\substack{k,p \\ k \neq p}} f_k f_p c_{k,\uparrow}^\dagger c_{-k,\downarrow}^\dagger c_{-p,\downarrow} c_{p,\uparrow} \tag{6}$$

with the single particle energies

$$\varepsilon_k \equiv -2t\big(\cos(k_x) + \cos(k_y)\big) - 4t'\big(\cos(k_x)\cos(k_y)\big)$$

and the form factor

$$f_k \equiv \cos(k_x) - \cos(k_y)$$

for modeling the d-wave interaction and $f_k = 1$ for the s-wave interaction. The model of equation (6) is superconducting in the BCS approximation. For the s-wave interaction superconductivity has been rigorously proven [26].

The ground state of the BCS-reduced models with s-wave and d-wave interaction for a fixed number of particles can be calculated without any approximations with the stochastic diagonalization technique [27–29]. This method we used to calculate the ground state of the BCS-reduced models in finite lattices. One disadvantage of the SD is the impossibility of calculating error bars of the physical expectation values like the ground state energy [27]. Details of the SD method are published in [27,29].

Figure 1 shows the $1/L_x$ scaling of for the J-model. For weaker interaction we would reach the same conclusion, the absence of superconductivity, as other authors in the case of the HM. Only the case $J = -0.25$ would be superconducting. Considering the susceptibility ($\chi_{\mathrm{d}}^{\mathrm{V}} \equiv L\bar{C}_{\mathrm{d}}^{\mathrm{V}}$) again for weaker interaction the divergence of $\chi_{\mathrm{d}}^{\mathrm{V}}$ is ambiguous.

The absolutely new approach is, that the conclusions are drawn from the corrections to scaling and not from the scaling alone. These corrections are due to the same kinetic part of the two Hamiltonians, which is the same in the BCS-reduced and the HM. Therefore the comparison of both models is possible. The use of the average of the CFs has been examined in [10]. Accordingly we have for each interaction U and system size L an effective J_{e} of the J-model. Only from the comparison of the J_{e} for several system sizes L we draw our conclusions about superconductivity.

Before we carry out this comparison, we have to circumvent a further complication in the HM. The values of the CFs $C_{\mathrm{d}}^{\mathrm{V}}(r)$ are extremely large for smaller distances $|r|$ [9,10,30] and therefore susceptible to the fluctuations of the numerical simulations. Indeed these fluctuations for smaller distances exceed the "plateau" value of the $C_{\mathrm{d}}^{\mathrm{V}}(r)$. As only the long range behavior is of interest for superconductivity we restrict the average vertex CF

$$\bar{C}_{\mathrm{s}}^{\mathrm{V,P}} \equiv \frac{1}{L_{\mathrm{c}}} \sum_{\substack{r \\ |r|>|r_{\mathrm{c}}|}} C_{\mathrm{s}}^{\mathrm{V}}(r) \tag{7}$$

to the distances $|r| > |r_{\mathrm{c}}|$. In equation (7) $|r_{\mathrm{c}}|$ is a critical distance and L_{c} is the number of points with $|r| > |r_{\mathrm{c}}|$ (for $r \in 1, \ldots, L$). Typically we choose $|r_{\mathrm{c}}| = 1.9$.

Performing PQMC simulations the projection parameter θ and the number m of Trotter-Suzuki slices have to be chosen adequately. In agreement with the literature, *e.g.* [11,22,23] we use $\theta = 8$ and $m = 64$.

We determine J_{e} in the following way: for the system parameters L, $\langle n \rangle \equiv (n_\uparrow + n_\downarrow)/L$ (with n_σ electrons with spin σ), t', and U we calculate $\bar{C}_{\mathrm{d}}^{\mathrm{V,P}}$ for the HM with PQMC. For the same set of parameters we tune J using the SD method to obtain the same value $\bar{C}_{\mathrm{d}}^{\mathrm{V,P}}$ in the J-model. This J is our effective interaction J_{e}.

A first test was carried out for the negative (attractive) HM, which is commonly believed to be superconducting (s-wave symmetry). Results in Figure 2 show an unique J_{e} for system sizes 6×6 to 12×12 and small deviations at 4×4. $|r_{\mathrm{c}}| = 1.9$ was chosen for this and all following cases. It should be mentioned, that the choice of $|r_{\mathrm{c}}|$ is not critical for the qualitative behavior of J_{e}.

We want to note, that on account of the use of the vertex CF (which is zero for $U = 0$) and consideration of the corrections to scaling it is possible to draw the conclusions even for weak interactions as $U = -0.5$.

In Figure 3 we return to the repulsive HM. For $U = 2$ and $t' = -0.22$ we again obtain as in the attractive case an unique J_{e} for system sizes 6×6 to 12×12. We notice a decrease for 16×16. The same effect occurs for the case $U = 1$. But for $t' = 0$ (the pure HM, $U = 2$) we find a constant J_{e} up to 16×16 (Fig. 3).

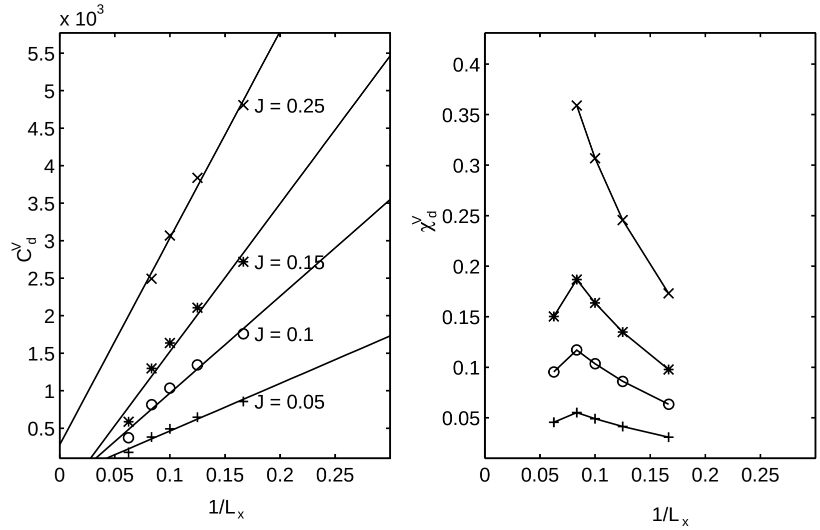

Fig. 1. Finite size scaling of the averaged (left, $\bar{C}_{\rm d}^{\rm V}$) and the cumulated (right, $\chi_{\rm d}^{\rm V}$) vertex CFs. The ground state of the BCS-reduced model with d-wave interaction was calculated with the stochastic diagonalization. The fillings of Table 1 and $t' = 0$ were used.

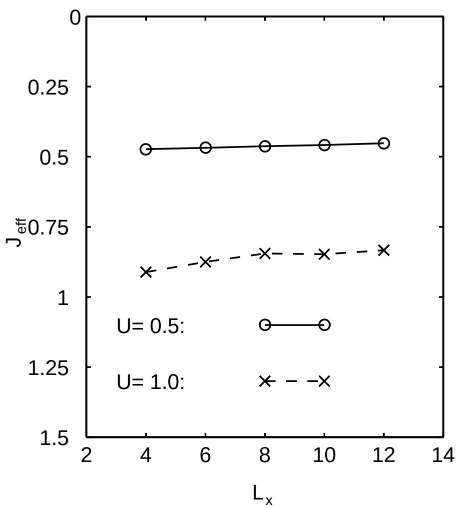

Fig. 2. Effective interaction $J_{\rm e}$ of the BCS-reduced model with s-wave interaction. The PQMC calculations were performed with $\theta = 8$ and $m = 64$ for the attractive tt'-HM with $\langle n\rangle$ and L of Table 1 and $t' = 0$.

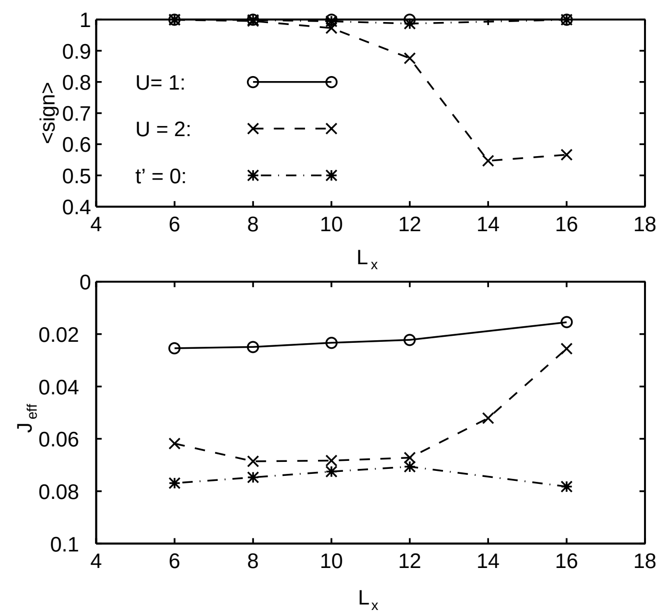

Fig. 3. Average sign $\langle\text{sign}\rangle$ (upper part) and effective interaction $J_{\rm e}$ (lower part) of the BCS-reduced model with d-wave interaction. The PQMC calculations were performed with $\theta = 8$ and $m = 64$ for the repulsive tt'-HM with $\langle n\rangle$ and L of Table 1. For the runs with the label $U = 1$ and $U = 2$ we choose $t' = -0.22$ and for the runs labeled with $t' = 0$ we use $t' = 0$ and $U = 2$.

This behavior is explained by the existence of different finite size gaps. For the small gaps in the $t' = -0.22$ case the simulations are only valid for relatively large projection parameters θ, which exceed our numerical possibilities. In Figure 4 we show the increase of $\bar{C}_{\rm d}^{\rm V,P}$ with various θ. In contrast the upper curve shows the leveling off in the $t' = 0$ case for a still moderate θ. This is caused by the relatively large finite size gap.

Therefore we conclude, that the deviation for $L = 16 \times 16$ in the $t' = -0.22$ system is due to insufficiently large θ in the simulation. The system does not reach the ground state properly. Larger θ are outside of the reach of methods. At this point we would like to mention that energy measurements are still rather insensitive to θ compared to the vertex CFs [13]. This is a rather important point as agreement in energy measurements was often used as evidence for the validity of a certain numerical method.

Considering again Figure 3 we conclude from the constant $J_{\rm e}(U)$ that our simulations show clear evidence for the existence of d-wave superconductivity in the HM.

The simulations had to be restricted to values $U \leq 2$ and system sizes up to 16×16 because of the convergence

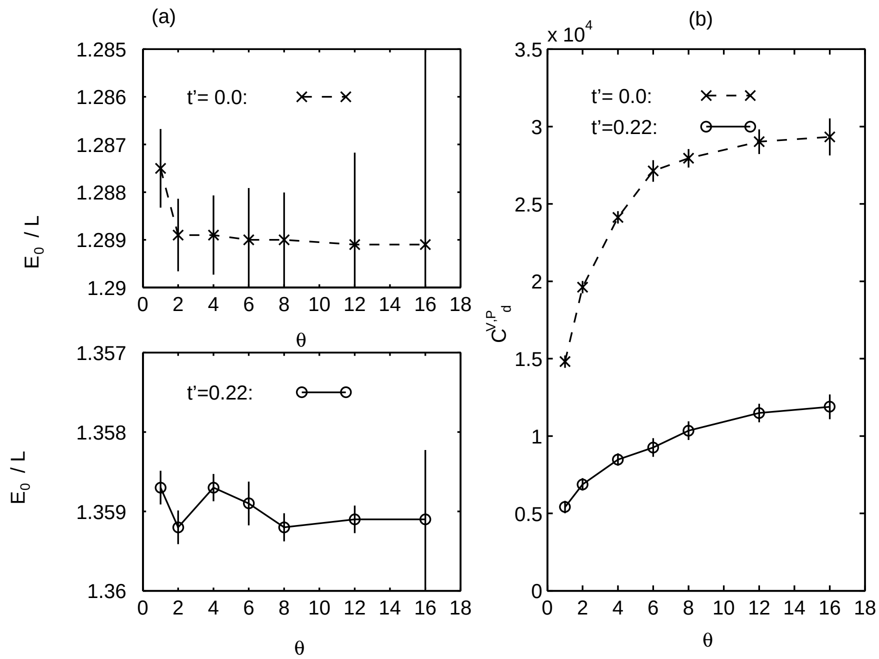

Fig. 4. The θ-scaling is plotted for the 16×16 system with the filling $n_\uparrow = n_\downarrow = 105$, the interaction $U = 1$ and $t' = -0.22$ (runs: $t' = -0.22$) and for the 16×16 system with the filling $n_\uparrow = n_\downarrow = 109$, the interaction $U = 2$ and $t' = 0$ (runs: $t' = 0$). The average sign $\langle \text{sign} \rangle$ is in both cases about one and $\theta/m = \tau = 0.125$. θ *versus* ground state energy per site, E_0/L (a) and θ *versus* the averaged vertex CF with $|r_c| = 1.9$, $\bar{C}_d^{V,P}$ (b).

problems of the PQMC method outside this parameter regime. This is clearly indicated by a dramatic break down of the average sign (Fig. 3). Figure 5 shows the regime of "safe" simulations below the shaded areas.

The effective interaction J_e leads to a superconducting T_c in the BCS-model [31]. The BCS-T_c has to be considered as at least a rough estimate and it does not include fluctuations in the two-dimensional system. Simulations for the attractive HM model by Schneider *et al.* [32] suggest that for the range of our interactions the deviation of the BCS-T_c and the real T_c of the repulsive HM is rather small.

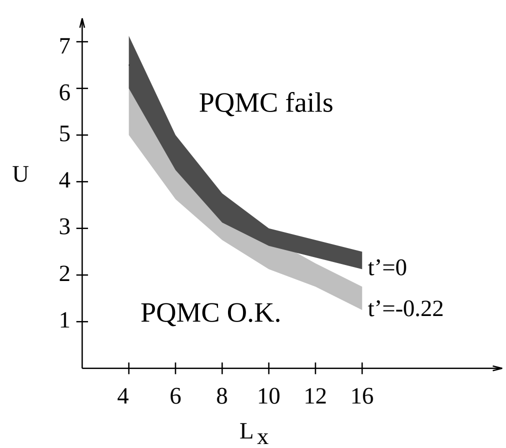

Fig. 5. Approximate limits (shadowed areas) of the PQMC for the tt'-HM with the filling $\langle n \rangle \approx 0.8$ and $t' = 0/t' = -0.22$.

For the $J_e \approx 0.07$ in Figure 3 ($U = 2$, $t' = -0.22$) we only obtain a very low $T_c \approx 1$ K, if we choose the energy scale $1t = 1$ eV. But in a 6×6 system we are able to calculate $U = 4$ with a sufficient large θ. For $t' = -0.22$ we find $J_e \approx 0.2$. This effective interaction leads $T_c \approx 30$ K. In contrast for $t' = 0$ we obtain $T_c \approx 3$ K.

The effective interaction $J_e \approx 0.2$ of $L = 6 \times 6$ agrees very well with a recently published 12×12 lattice [11]. The difference of T_c can be explained by the closeness of the Van Hove singularity in the $t' = -0.22$ case [10]. Larger values of $\bar{C}_d^{V,P}$ for $U = 6$ and $U = 8$ as suggested by 4×4 exact diagonalization results may lead to a dramatic increase of T_c. But we do not want base this decision on 4×4 lattice sizes. The conclusion of [11] that in the HM the superconducting correlations vanish for larger U and larger L is not valid. They decay only to a very small value. The errorbars of $C_d(r)$ in [11] are about ten times larger than the value of $\bar{C}_d^V$ for $U = 4$ and $L = 16 \times 16$ predicted by our J-model simulations with the effective interaction $J_e \approx -0.2$, which is obtained by the comparison of the J-model and the HM in smaller system sizes L.

In conclusion we provide clear evidence for the existence of d-wave superconductivity in the HM. For $U = 4$ we obtain a $T_c \approx 30$ K. Therefore the single band HM has to be considered as a serious candidate for the explanation of high T_c superconductivity.

One main conclusion of our simulations (Fig. 5) is, that all results published for $U \geq 4$ and $L \geq 8 \times 8$ exhibit incorrect data. Therefore conclusions concerning superconductivity drawn from these simulations are incorrect.

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