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Short Communication

Numerical simulation of the double layer Hubbard model


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Abstract. — We have carried out Quantum Monte Carlo studies to investigate the double layer Hubbard model using the groundstate projector formalism. Evidence for off diagonal long range order in the nodeless d-wave pairing channel is provided. It is emphasized that the Projector Quantum Monte Carlo method has the potential to detect superconducting mechanisms in strongly correlated electron systems, which are not treatable by standard analytic methods. The Monte Carlo technique provides useful information about systems much larger than those accessible for exact diagonalization methods.

It is commonly accepted that the CuO$_2$-planes play an essential role in the understanding of high temperature superconductivity [1]. Various models have been proposed to describe the properties of these planes: 1-Band Hubbard model [2,3], the t-J model [4], the Emery model [5,6] and the “apex-oxygen” model [7,8]. Numerical simulations based on the Quantum Monte Carlo method (QMC) during the recent years mainly provided evidence against superconductivity for these models except the “apex-oxygen” model which considers additional phononic degrees of freedom. Superconductivity within the group of purely electronic models is still controversially discussed; evidence only exists for the unrealistic negative-U Hubbard model [9].

It should be noted that the above mentioned simulations almost exclusively concentrated on single layer models. We simulated double layer structures first in the context of the apex oxygen model to explain the increase of $T_c$ with growing number of immediatly adjacent CuO$_2$-layers. Then our interest shifted to purely electronic structures without a coupling to phononic excitations. The original idea to consider the double layer case goes back to Anderson and Schrieffer [3].

Bulut et al. [12] as well as Dagotto et al. [13] discussed the possibility of nodeless d-wave pairing in a purely electronic double layer model. They concluded that their results are compatible with experimental findings which so far were only explained in terms of (extended-) s-wave superconductivity, but they were unable to reach low enough temperatures to detect superconductivity in their QMC simulations.
Here we want to give clear evidence in favour of nodeless d-wave superconductivity in the double layer Hubbard model using the Projector Quantum Monte Carlo method (PQMC). The same well-tested algorithm has been used to detect the superconducting properties of the “apex-oxygen” model. Until now there is no evidence in single layered purely electronic models. By means of PQMC [10] we are able to investigate the single layered purely electronic models. The orthogonalization technique originally proposed by Sorella et al. [14] helped us to stabilize the algorithm thus avoiding the well known difficulties concerning the famous “minus-sign” problem for fermionic systems [10,15].

The model Hamiltonian reads as

$$\mathcal{H} = -t \sum_{i,j,\sigma} \left( c_{i\sigma}^\dagger c_{j\sigma} + \text{h.c.} \right) - t_\perp \sum_{i,j,\sigma} \left( c_{i\sigma}^\dagger c_{j\sigma} + \text{h.c.} \right) + U \sum_i n_{i\uparrow} n_{i\downarrow}. \quad (1)$$

The first part of the Hamiltonian describes the in-plane particle motion, whereas the second term concerns the hopping of fermions between the layers. We consider apart from the usual in-plane pair correlation functions [11] the nodeless d-wave case (Fig. 1).

$$\chi(l) = \frac{1}{N} \sum_i \langle 0 | \Delta^\dagger(i) \Delta(i+l) | 0 \rangle \quad (2)$$

measures the correlation between two Cooper pairs separated by a distance $l$;

$$\Delta^\dagger(i) = c_{i,\uparrow}^\dagger c_{i,\downarrow}^\dagger$$

denotes the “cooper pair creator” with one charge carrier in layer 1 and the other in layer 2, e.g. the cooper pair spans over the two layers, as shown in figure 1.

Fig. 1. — Schematic definition of the nodeless d-wave pairing correlation symmetry; the position of the fermionic creation and annihilation operators in the two-layer system is indicated.
To detect the effective interaction between the carriers within the cooper pair we focus our attention on the vertex correlation function without any residual quasi-particle interaction

$$\chi_{\text{vertex}}(l) = \chi(l) - \langle 0 | c_{i,11}^\dagger c_{i,22} | 0 \rangle \langle 0 | c_{i,11}^\dagger c_{i,22}^\dagger | 0 \rangle. \quad (5)$$

From the sign of the vertex function it is possible to conclude whether we deal with an attractive or repulsive interaction between the particles. According to Yang [16] the condition for off diagonal long range order (ODLRO) in a system is

$$\chi_{\text{vertex}}(l) \to c_m \quad \text{for} \quad l \to \infty, \quad (6)$$

with a nonzero $c_m$ as a long-range plateau value.

The described concept of ODLRO is directly related to superconductivity. Figure 2 shows in a semilogarithmic plot our vertex correlation function $\chi_{\text{vertex}}(l)$ versus distance $l$. The simulations were carried out for an (8x8x2) single band Hubbard model; the parameters are $U/t = 8$, $t_\perp/t = 0.6$, with $t$ as an energy unit. We considered the case of $\delta = 15\%$ doping (i.e. 0.15 holes per site) corresponding to a closed shell case (see [7,10]). There is no severe "minus-sign" problem, as shown in figure 3. Results for a smaller (6x6x2)-System with equivalent parameters show similar behavior.

Returning to figure 2 we notice an exponential decay of $\chi_{\text{vertex}}(l)$ for small distances, giving us a very short correlation length. Then the vertex reaches obviously the mentioned plateau value $c_m \approx 10^{-5}$

![Figure 2](image_url)  

Fig. 2. — Semilogarithmic plot of the nodeless d-wave vertex correlation function versus cooper pair distance in the two-layer Hubbard model. Notice the exponential decay within three lattice spaces and the long range finite plateau-value. Parameters: (8x8x2)-Hubbard model, $t = 1$ (serves as energy unit), $t_\perp = 0.6t$, $U/t = 8$, projection parameter $\Theta = 8$, doping $\delta = 15\%$ corresponding to a closed shell case [7,10]. We show a typical errorbar for the value with the largest distance.
We are aware of the fact that larger lattices are essential to support our claim, but present CPU-time requirements did not allow us further investigations; they are planned for the future. Furthermore the choice of \( t_{\perp} = 0.6t \) is probably too high for the most interesting case of high temperature superconductivity. Lower, more realistic values of \( t_{\perp} \) are expected to lead to considerably higher consumption of CPU-time. To produce the presented results for the \((8 \times 8 \times 2)\) single band Hubbard model an amount of more than 300 hours CPU-time on a Cray-YMP was necessary.

In conclusion we want to state that we detected ODLRO in the nodeless d-wave pairing channel. The importance of the described scenario for high temperature superconductivity is still an open question. As the value for the long-range plateau is lower than in the "apex-oxygen" case one would expect that an additional "booster" mechanism, perhaps in form of phononic degrees of freedom, leads to a remarkable higher critical temperature. Further investigations are currently under way.

In particular the case of a double layer Emery model, which will consume considerably more computer time, also seems to show ODLRO in that pairing channel. Larger lattices have to be studied, results will be published in the near future.

![Figure 3. Average sign as a function of Monte Carlo steps; the high value indicates that there is no severe minus sign problem. The simulation was carried out over more than three million Monte Carlo steps.](image)

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