QUANTUM MONTE CARLO SIMULATIONS FOR HIGH-\(T_c\) MODELS

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Numerical simulations were carried out using a projector quantum Monte Carlo method pioneered by Sorella et al. Ground state energies are presented for the single band Hubbard model for system sizes 4 \(\times\) 4 to 8 \(\times\) 8. The Hubbard model coupled to a two-level system (e.g. bridging oxygen) was also studied. Enhancement of superconducting susceptibilities indicates the possibility of high-\(T_c\) superconductivity.

The projector quantum Monte Carlo method recently introduced by Sorella et al. [1] has proved to be a powerful tool to simulate the Hubbard model since [2].

\[ \mathcal{H} = -t \sum_{\langle i,j \rangle} c_i^\dagger c_j + H.c. + U \sum_i n_i n_{i+1}. \]  

(1)

In this short review, we first present results on the ground state energies of Hamiltonian (1) for 4 \(\times\) 4 systems with various numbers of holes and different values for repulsive interaction \(U\) (fig. 1). We can see that \(U\) is a straight line up to \(U = 4\), after which there is a clearly negative curvature. This means that we have no binding energy for bringing additional holes into the system. For \(U \geq 6\), we even see a clear repulsion of the holes. The simple fact is that it costs energy to insert an additional hole into the system. Figure 2 shows the case for \(U = 8\) with additional system sizes up to 8 \(\times\) 8. We notice that the tendency towards repulsion of holes is even more pronounced for larger system sizes. Figure 3 shows the case for \(U = 4\), where again no binding is seen. Figure 4 shows the hole concentration regime for a 6 \(\times\) 6 system with \(U = 8\).

Although our system sizes are rather limited, we consider our results evidence against high-\(T_c\) superconductivity in the Hubbard model, especially on the basis of the short coherence lengths in the actual materials.

To approach superconductivity, we followed the suggestion by Müller to couple a two-level system to the Hubbard model [3] because of the bridging oxygen:

\[ \mathcal{H} = \text{Hubbard} + e \sum_i n_i \sigma_i^z + \Omega \sum_i \sigma_i^x. \]  

(2)
The two-level system is represented by additional spin $\sigma'_c$.

Considering the case $\varepsilon = 1$, $\Omega = 0.5$ and $U = 8$, we see for the superconducting oxide and nearest-neighbor susceptibility,

$$\chi_0(n) = \frac{1}{N} \sum_{i,j} c^+_i c^+_j c_i (c_{i+1}) c_j (c_{j+1})$$

(3)

an increase with system size for $4 \times 4$ to $8 \times 8$ compared to the pure case (figs. 5 and 6). We interpret these preliminary findings as a possible explanation of high-$T_c$ superconductivity.

References