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].

\[ \mathcal{H} = -t \sum_{\langle i,j \rangle} \hat{c}^+_i \hat{c}^+_j + \text{H.c.} + U \sum_i n_i n_{i+1}. \]  

(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,

$$\chi_0(n) = \frac{1}{N} \sum_{i,j \neq i} c_{i\uparrow}^+ c_{i\downarrow}^+ c_{j\uparrow} c_{j\downarrow} ,$$

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

