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].

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

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:

\[
\mathcal{H} = \text{Hubbard} + e \sum_i n_i \sigma_i^x + \Omega \sum_i \sigma_i^z. \tag{2}
\]
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,

\[
\chi_{\sigma_0}(n) = \frac{1}{N} \sum_{i,j} \epsilon_{i}^c c_{i+1}^c | \epsilon_{i}^c c_{i+1}^c |,
\]

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

