University of Groningen

Quantum Monte Carlo Simulations for High-Tc Models

Morgenstern, I.; Linden, W. von der; Frick, M.; Raedt, H. De

Published in:
Physica B: Condensed Matter

DOI:
[10.1016/0921-4526\(90\)90294-5](https://doi.org/10.1016/0921-4526(90)90294-5)

IMPORTANT NOTE: You are advised to consult the publisher's version (publisher's PDF) if you wish to cite from it. Please check the document version below.

Document Version
Publisher's PDF, also known as Version of record

Publication date:
1990

[Link to publication in University of Groningen/UMCG research database](#)

Citation for published version (APA):

Morgenstern, I., Linden, W. V. D., Frick, M., & Raedt, H. D. (1990). Quantum Monte Carlo Simulations for High-Tc Models. *Physica B: Condensed Matter*, 163(1). [https://doi.org/10.1016/0921-4526\(90\)90294-5](https://doi.org/10.1016/0921-4526(90)90294-5)

Copyright

Other than for strictly personal use, it is not permitted to download or to forward/distribute the text or part of it without the consent of the author(s) and/or copyright holder(s), unless the work is under an open content license (like Creative Commons).

The publication may also be distributed here under the terms of Article 25fa of the Dutch Copyright Act, indicated by the "Taverne" license. More information can be found on the University of Groningen website: <https://www.rug.nl/library/open-access/self-archiving-pure/taverne-amendment>.

Take-down policy

If you believe that this document breaches copyright please contact us providing details, and we will remove access to the work immediately and investigate your claim.

Downloaded from the University of Groningen/UMCG research database (Pure): <http://www.rug.nl/research/portal>. For technical reasons the number of authors shown on this cover page is limited to 10 maximum.

QUANTUM MONTE CARLO SIMULATIONS FOR HIGH- T_c MODELS

I. MORGENSTERN^a, W. VON DER LINDEN, M. FRICK and H. DE RAEDT

IBM Research Division, Zurich Research Laboratory, 8803 Rüschlikon, Switzerland

^aInstitute of Physics, University of Zurich, Schönberggasse 9, 8001 Zurich, Switzerland

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 4×4 to 8×8 . 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],

$$\mathcal{H} = -t \sum_{(i,j)} c_i^\dagger c_j + \text{H.c.} + U \sum_i n_{i\uparrow} n_{i\downarrow}. \quad (1)$$

In this short review, we first present results on the ground state energies of Hamiltonian (1) for 4×4 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

Fig. 1. Groundstate energies for 4×4 systems for various U against number of holes.

Fig. 2. Groundstate energies for 4×4 , 6×6 , 8×8 for $U = 8$. Repulsion between holes!

system sizes up to 8×8 . 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 6×6 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:

$$\mathcal{H} = \text{Hubbard} + \varepsilon \sum_i n_i \sigma_i^z + \Omega \sum_i \sigma_i^x. \quad (2)$$

Fig. 3. Groundstate energies for 4×4 and 6×6 for $U = 4$. Fig. 4. Groundstate energies for 6×6 and $U = 8$. Whole range of hole concentration.

The two-level system is represented by additional spin σ'_i .

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

$$\chi_0(n) = \frac{1}{N} \sum_{\substack{i,j \\ (i \neq j)}} c_{i\uparrow}^\dagger c_{i(+1)\downarrow}^\dagger c_{j\uparrow} c_{j(+1)\downarrow}, \quad (3)$$

an increase with system size for 4×4 to 8×8 compared to the pure case (figs. 5 and 6). We interpret

Fig. 5. Two-level system. Onsite s-wave susceptibility (eq. (3)) shows increase with system size. No increase for pure Hubbard model.

Fig. 6. Similar to fig. 5 for extended s-wave susceptibility.

these preliminary findings as a possible explanation of high- T_c superconductivity.

References

- [1] S. Sorrella, E. Tosatti, S. Baroni, R. Car and M. Parrinello, in: Proc. Adriatic Research Conf. Towards the Theoretical Understanding of the High- T_c Superconductors, S. Lundqvist, S. Sorella, S. Baroni, R. Car and M. Parrinello, eds., Europhys. Lett. 8 (1989) 663.
- [2] M. Imada and Y. Hatsujai, preprint.
- [3] I. Morgenstern, Int. J. Mod. Phys. B 1 (1988) 975.