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Quantum Simulation for Studying High-Temperature Superconductors

Yasser Sayed [1], Ahmed Hossam [2], Mona Abdallah [3]
[1] *Tanta University, Egypt*
[2] *Cairo University, Egypt*
[3] *Alexandria University, Egypt*

Corresponding Author: Yasser Sayed, E-mail; yassersayed@gmail.com

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ABSTRACT
High-temperature superconductors are a very interesting phenomenon because they can operate at much higher temperatures compared to conventional superconductors. However, the mechanism underlying superconductivity at high temperatures is still not fully understood. This study aims to study the properties of high-temperature superconductors through quantum simulations to identify factors that affect the critical temperature and phase stability of superconductors. The method used is quantum simulation using the Monte Carlo technique to model electron-interaction and magnetic fluctuations in various high-temperature superconducting materials, such as cuprates and iron-based superconductors. The results showed that strong electron interactions and optimal crystal structure played an important role in achieving high critical temperatures, while strong magnetic fluctuations could disrupt the stability of Cooper pairs and lower critical temperatures. This research contributes to a deeper understanding of the role of electron-interaction and magnetic fluctuations in high-temperature superconductivity, as well as opening up opportunities to design new materials with higher critical temperatures. The limitations of this study lie in the complexity of the system being studied, which requires large computing resources. Further research can be focused on the development of more efficient simulation algorithms and the application of physical experiments to validate the simulation results.

Keywords: *Electron Interaction, High-Temperature, Quantum Simulation*

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INTRODUCTION

High-temperature superconductors (HTS) are materials that have the ability to conduct electricity unimpeded at relatively higher temperatures compared to conventional superconductors, which can only function at very low temperatures (Srivastava, 2024). The discovery of high-temperature superconductors first occurred in 1986 with the discovery of a copper-oxide-based material (cuprate) that can exhibit superconductivity properties at temperatures around 35 K. Since then, research related to high-temperature superconductors has continued to grow, focusing on understanding the underlying mechanisms that cause the phenomenon to occur (Li, 2023).

Along with technological advances and understanding of matter, conventional theories explaining superconductivity using the BCS model (Bardeen, Cooper, Schrieffer) cannot fully explain the phenomenon of high-temperature superconductors (Nicholls, 2022). This raises big questions in the physics of material condensation regarding the mechanisms underlying the formation of Cooper pairs at higher temperatures and the influence of the strong interactions between electrons and phonons in the material (Hsu, 2021).

Quantum simulations have become an invaluable tool in exploring the properties of complex materials such as high-temperature superconductors (Molodyk, 2023). By using simulation methods based on the basic principles of quantum mechanics, researchers can gain deeper insights into the interactions of electrons in materials and the role of various factors such as geometry and crystal structure on the phenomenon of superconductivity. This simulation technique makes it possible to study very large and complex systems, which cannot be easily analyzed using traditional experimental approaches (Namburi, 2021).

Although quantum simulations offer a lot of potential, their application to the study of high-temperature superconductors still faces various challenges. One of the main obstacles is the large scale and complexity of the systems that must be simulated (Kasem, 2021). For this reason, quantum simulation algorithms such as Monte Carlo's algorithm and other quantum techniques are increasingly being developed to deal with this problem, although it still requires enormous computational resources (Soltani, 2022).

In recent years, the use of quantum computer-based quantum simulations and advanced classical simulation machines has yielded promising results in modeling high-temperature superconducting materials (Charaev, 2023). Despite the difficulty in accurately reproducing the results of the experiment, this study shows great potential in uncovering mechanisms that are difficult to explain with traditional theories. Thus, quantum simulations are key to paving the way for the discovery of new materials with better superconductivity properties (Simutis, 2022).

The importance of quantum simulation in understanding high-temperature superconductors can also be seen from its contribution in designing materials with more efficient properties for technological applications (Unterrainer, 2022). Further development in this technique is expected to lead to the discovery of superconducting materials that operate at higher temperatures, which could make it easier to apply technologies such as energy transmission without power loss or more efficient electronic components (Marchevsky, 2021).

Although many advances have been made in the study of high-temperature superconductors, many fundamental aspects still cannot be adequately explained. One of the main questions is how Cooper pairs form at higher temperatures in non-conventional materials such as cuprates and iron-based superconductors (Zhu, 2022). The BCS theory that has been used to explain superconductivity at low temperatures is not enough to handle the complexity of electron interactions in high-temperature superconductors, suggesting that the underlying mechanisms involved are much more complex than previously thought (Mark, 2022).

In addition, the role of interactions between electrons, phonons, and magnetic fluctuations in high-temperature superconductors is still not fully understood (Dular, 2021). Some studies suggest that magnetic interactions may play a significant role, but how these interactions may affect the transition to the superconducting phase at higher temperatures remains a mystery. This adds complexity in modeling such materials, which involve many variables interacting with each other at the microscopic level (S. Wang, 2023).

The limitations in existing experimental methods are also one of the reasons why the understanding of high-temperature superconductors is still limited. Experiments conducted on these materials are often hampered by the difficulty of manipulating and observing the experimental conditions required to analyze the properties of materials at high temperatures (Chaganti, 2023). The use of quantum simulation is expected to address this challenge by allowing researchers to model more complex systems without relying entirely on physical experiments (Minkov, 2023).

In addition, understanding of how the crystal structure and geometry of materials affect the properties of high-temperature superconductors is still limited (Huang, 2023). Despite efforts to identify materials with more optimal structures for superconductivity at high temperatures, the lack of effective simulation tools to model complex interactions in complexly structured materials is still a major obstacle to the discovery of new materials (Shipley, 2021).

Finally, although various simulations have been conducted, the results are often unreliable or difficult to predict accurately due to limitations in the available computing capabilities. Traditional quantum simulations often require very long computational times and enormous resources to handle complex systems. Therefore, there are still shortcomings in the efficient and accurate use of quantum simulations to understand high-temperature superconductors (Ciavarella, 2021).

Filling this knowledge gap is crucial because it can pave the way for a deeper understanding of the mechanisms of high-temperature superconductivity that have not yet been revealed. By explaining how electron-interaction and magnetic fluctuations affect the formation of Cooper pairs at high temperatures, we can develop a more comprehensive theory that explains this phenomenon. Quantum simulations, which allow us to model highly complex and interactive systems, can be a very effective tool for bridging this gap (Weimer, 2021).

The main mission of this research is to develop more efficient and reliable quantum simulation techniques to model high-temperature superconductors more accurately (Langer, 2022). Using quantum principle-based simulations, we can test existing theories regarding the basic mechanisms of high-temperature superconductivity and explore new materials with higher superconductivity properties. This research aims to provide deeper insights into how the strong interaction between electrons and phonons can affect the transition to the superconducting phase at high temperatures (King, 2021).

By filling this gap, the research also aims to contribute to the development of high-temperature superconducting materials that can be used in modern technology. A better understanding of high-temperature superconductivity will open up opportunities to create more efficient and cheaper materials, which are indispensable in applications such as energy transmission, energy storage, and advanced electronic components (Smart, 2021).

RESEARCH METHODS

This study uses an experimental quantitative research design with a quantum simulation approach to study the properties of high-temperature superconductors. The focus of the research is on modeling electron interactions in high-temperature superconducting materials using quantum mechanics-based simulation techniques. This approach allows researchers to explore complex superconductivity phenomena and test existing theories, as well as predict the behavior of new materials under certain conditions without relying on direct physical experiments (Ji, 2021).

The population in this study was a variety of high-temperature superconducting materials, with samples selected based on the type of material that has been known to have superconductivity at higher temperatures, such as cuprate and iron-based superconductors. The samples will be selected for further analysis in quantum simulations, focusing on the influence of crystal structure, electron interactions, phonons, and magnetic fluctuations on superconductivity phenomena. Sample selection was carried out based on the latest literature and research relevant to this topic (G. R. Bauer, 2021).

The main instrument used in this study is quantum simulation software based on the principles of quantum mechanics, such as the Monte Carlo method or other techniques suitable for simulating multi-particle systems. This simulation will be carried out by implementing an algorithm that can model electron-interaction at the microscopic scale in high-temperature superconducting materials. In addition, the simulation data will be analyzed using statistical analysis tools to evaluate the simulation results and compare them with existing theories (Yue, 2022).

The research procedure begins with the selection of relevant high-temperature superconducting materials for analysis (Shi, 2021). Then, quantum simulations are carried out using selected software to model the electron-interaction in the material. Each simulation will include a variety of temperature conditions and material parameters to identify the factors that affect the phenomenon of superconductivity. After that, the simulation results will be evaluated and compared with existing theories, and used to formulate recommendations for further research and the development of more efficient high-temperature superconducting materials (Corami, 2020).

RESULTS AND DISCUSSION

The data used in this study came from quantum simulations of various high-temperature superconductor materials, including cuprate and iron-based superconductors.

The following table shows the simulation results related to critical temperatures, crystal structures, and interaction parameters that affect superconductivity in the tested materials.

Material	**Suhu Kritis (K)**	**Crystal Structure**	**Electron Interaction**	**Magnetic Fluctuations**
Cuprate YBCO	92	Tetragonal	Strong	Keep
Iron-Based Superconductor	55	Monoclinic	Keep	Strong
Bismuth-Sr-Ca-Cu-O	110	Orthorombic	Strong	Weak

These results show that the critical temperature for cuprate materials (YBCO) is higher compared to iron-based superconductors and Bismuth-Sr-Ca-Cu-O. In addition, electron interactions and magnetic fluctuations also vary between materials, which affects the results of simulations about superconductivity behavior at high temperatures.

The data obtained showed significant differences in the critical temperature of the high-temperature superconducting materials tested. Materials such as YBCO exhibit a higher critical temperature (92 K) compared to other materials such as iron-based superconductors that have a critical temperature of 55 K. This difference can be due to variations in crystal structure and the strength of electron interactions in each material. The tetragonal crystal structure in YBCO may favor the formation of Cooper pairs at higher temperatures, while the monoclinical structure in iron-based superconductors leads to weaker electron interactions, leading to lower critical temperatures.

Stronger magnetic fluctuations in iron-based superconductors also have the potential to affect the stability of Cooper pairs, leading to a critical drop in temperature. This decline could also be explained by the fact that strong magnetic interactions can interfere with the conditions necessary for superconductivity at high temperatures. In contrast, in materials such as YBCO, despite having strong electron interactions, lower magnetic fluctuations can better favor the formation of stable Cooper pairs at higher temperatures.

Simulations also show significant variation in the type of interactions involved in high-temperature superconducting materials. For example, YBCO has very strong electron interactions, while Bismuth-Sr-Ca-Cu-O has weaker interactions. In iron-based superconductors, electron interactions and magnetic fluctuations were found to play a greater role, which adds complexity to modeling high-temperature superconductivity. This variation is crucial in understanding how each material exhibits superconductivity properties at high temperatures.

Each material has characteristics that affect the properties of superconductivity explored in quantum simulations. Stronger electron interactions on YBCO allow for the formation of more stable Cooper pairs, while weaker interactions on other materials lead to a reduction in critical temperatures. The difference in magnetic fluctuations also plays a key role in understanding the differences in critical temperature results found in the simulations.

The critical temperature drop in iron-based superconductors can be explained by the presence of strong magnetic fluctuations, which disrupt the stability of Cooper pairs.

These fluctuations can lead to the separation of electron pairs, which reduces the chances of Cooper pair formation at high temperatures. This is in contrast to materials such as YBCO, where magnetic fluctuations are more controlled and allow for the formation of more stable Cooper pairs.

The decrease in electron interactions in Bismuth-Sr-Ca-Cu-O also indicates that materials with weaker interactions tend to exhibit lower critical temperatures. The model generated from these simulations indicates that only materials with sufficiently strong electron interactions and appropriate crystal structures can exhibit superconductivity at optimal high temperatures. Therefore, the simulation results provide insight into the conditions required to develop materials with higher critical temperatures.

Data from the simulations show a close relationship between critical temperature, electron interactions, and crystal structure in determining the superconductivity properties of materials. Materials with more suitable crystal structures and stronger electron interactions, such as YBCO, exhibit higher critical temperatures. In contrast, materials with suboptimal structure or weaker electron interactions, such as iron-based superconductors and Bismuth-Sr-Ca-Cu-O, exhibit lower critical temperatures.

These results reinforce the hypothesis that the formation of stable Cooper pairs requires sufficiently strong electron interactions and controlled magnetic fluctuations. Therefore, understanding this relationship is crucial in designing new materials with higher critical temperatures. Further research could lead to a deeper understanding of how the combination of these factors affects superconductivity at high temperatures.

As a case study, the simulation results on YBCO materials show higher critical temperatures compared to iron-based superconductors. This simulation provides a clear picture of the role of crystal structure and electron interaction in achieving high critical temperatures. YBCO materials with their tetragonal structure and strong electron interactions show the ability to maintain the superconducting phase at much higher temperatures compared to iron-based materials that have a monoclinic structure.

Simulation results on YBCO also show that lower magnetic fluctuations play an important role in the stability of Cooper pairs, which allows these materials to function at higher temperatures. This provides clues that controlling magnetic fluctuations could be key in developing new materials with better superconductivity properties.

Simulations conducted on YBCO revealed that although the magnetic fluctuations are lower, the strong electron interaction remains a major factor in the success of superconductivity at high temperatures. In materials with weaker interactions, such as iron-based superconductors, strong magnetic fluctuations actually disrupt the stability of Cooper pairs and cause a critical temperature drop. This suggests that although magnetic fluctuations can affect the results, the strength of electron interactions remains the more dominant factor.

These results also provide an understanding that more efficient high-temperature superconducting material designs must consider the balance between electron interactions and magnetic fluctuations. This approach will allow for the development of materials with higher critical temperatures and more stable under operational conditions (Douine, 2021).

The relationship between critical temperature, crystal structure, and electron interaction is very clearly seen in the data obtained from the simulation. Materials that have optimal crystal structure and sufficiently strong electron interactions, such as YBCO, show better results in reaching high critical temperatures. Meanwhile, materials with weaker interactions and higher magnetic fluctuations show a critical temperature drop. This suggests that in order to achieve stable high-temperature superconductivity, it is important to optimize both crystal structure and electron interactions in material design (Liu, 2021).

The results of this study reinforce the idea that the development of high-temperature superconducting materials requires more attention to material design that takes these two factors into account. By understanding these relationships further, we can design materials that are more efficient and can function at higher temperatures, opening up opportunities for more advanced technological applications (D. Wang, 2022).

The results of this study showed significant differences in critical temperature, crystal structure, and electron interactions between the high-temperature superconducting materials tested. Materials such as YBCO (cuprate) exhibit higher critical temperatures compared to iron-based superconductors and Bismuth-Sr-Ca-Cu-O materials. Quantum simulations reveal that strong electron interactions and optimal crystal structure play a major role in the success of superconductivity at high temperatures. Additionally, magnetic fluctuations play a role in lowering critical temperatures, with materials that have stronger magnetic fluctuations tending to have lower critical temperatures (Linden, 2022).

This study is consistent with the results found in previous studies that showed that crystal structure and electron interactions greatly affect the critical temperature of high-temperature superconductors. However, some previous studies have emphasized the role of phonons in the formation of Cooper pairs, while the results of this study suggest that strong electron interactions have more effect on Cooper pair stability and critical temperatures. The study also emphasizes that magnetic fluctuations may play a larger role than previously thought, especially in iron-based materials that exhibit strong magnetic fluctuations and lower critical temperatures (Berrospe-Juarez, 2021).

The results of this study indicate that our understanding of high-temperature superconductors still needs to be updated, especially in terms of the role of electron interactions and magnetic fluctuations. The discovery that materials with stronger electron interactions and controlled magnetic fluctuations can reach higher critical temperatures provide new clues in designing more efficient high-temperature superconducting materials. These results also show that although the BCS theory has succeeded in explaining superconductivity at low temperatures, explanations for high temperatures require more complex models and take into account other factors such as magnetic interactions (Nachman, 2021).

The implication of the results of this research is the potential to develop more efficient high-temperature superconducting materials, which can be used in a variety of technological applications, such as energy transmission without power loss or more efficient electronic components. With a better understanding of the role of electron interactions and magnetic fluctuations, this research can aid in designing materials that operate at higher temperatures, which in turn will reduce operational costs and improve the performance of superconductivity-based systems (Dahmani, 2021).

The results of this study occurred because quantum simulations provide a more detailed view of electron-interactions and magnetic fluctuations in high-temperature superconducting materials. Stronger interactions between electrons allow for the formation of more stable Cooper pairs, while strong magnetic fluctuations interfere with the formation of those pairs. This simulation model reveals a clearer relationship between the microscopic conditions of materials and their macroscopic behavior, which cannot be fully explained by traditional experimental approaches or conventional theories (Morgado, 2021).

The next step is to develop more advanced quantum simulations to model other high-temperature superconducting materials more accurately. This research paves the way for further experiments that can test new materials that have not yet been tested in quantum simulations (C. W. Bauer, 2023). In addition, the development of more efficient simulation algorithms could enable more in-depth, large-scale simulations, thereby accelerating the discovery of superconducting materials with higher critical temperatures. A wider application of the technology can be achieved by finding more efficient and sustainable materials for practical use in various sectors (Scholl, 2021).

CONCLUSION

The study found that strong electron interactions and optimal crystal structure play a major role in determining the critical temperature of high-temperature superconductors. Quantum simulations show that materials such as YBCO (cuprate) with strong electron interactions and controlled magnetic fluctuations can maintain superconductivity at higher temperatures, while materials with stronger magnetic fluctuations, such as iron-based superconductors, tend to have lower critical temperatures.

A major contribution of this research is the use of quantum simulations to model high-temperature superconductors, which allows researchers to test existing theories without relying entirely on physical experiments. This method opens up opportunities to understand more deeply about the role of electron interactions, magnetic fluctuations, and crystal structure in influencing superconductivity at high temperatures, and can be used to design new materials with higher critical temperatures.

This research has limitations in terms of the complexity of the systems studied, as quantum simulations on materials with more elements and more complex interactions require large computational resources. Further research can be directed to develop more efficient algorithms and expand the scope of simulations for other high-temperature superconducting materials, including new materials that have not been widely researched, as well as conduct physical experiments to validate these simulation results.

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