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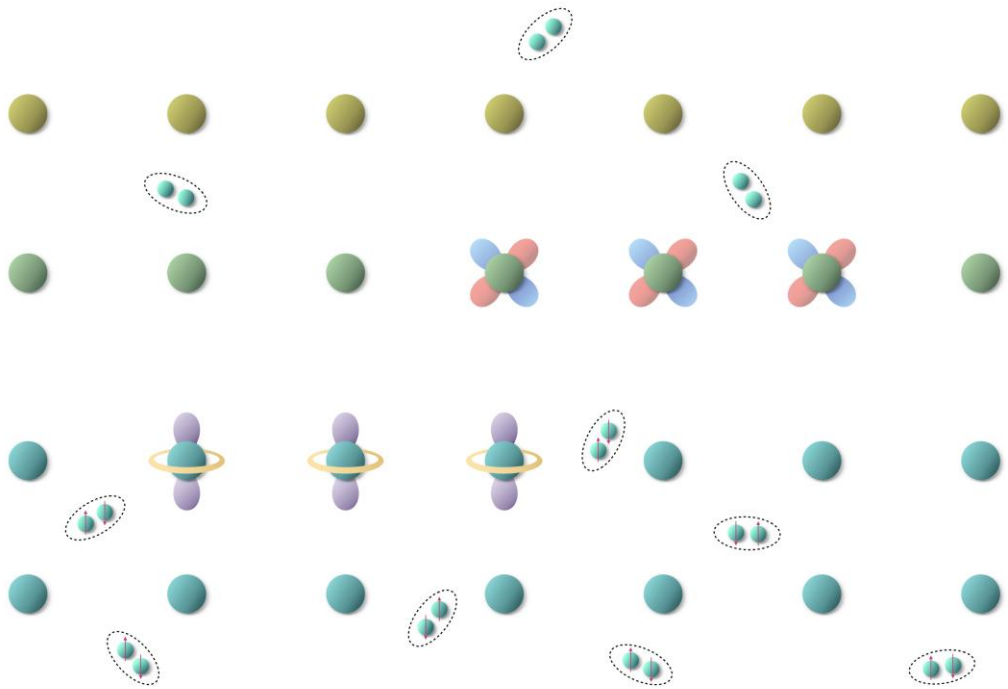
PRESS RELEASE

Finding the right combination: new simulations in the search for topological superconductors

A novel computational approach developed at SISSA makes it possible to realistically and efficiently simulate the proximity effect between materials, opening up new possibilities for research into topological superconductors and their potential applications in quantum computing. The paper has been selected as an Editors' Suggestion by the journal *Physical Review Research*



Trieste, 15 September 2026

A new theoretical and computational approach developed by a group at SISSA makes it possible to realistically and predictively simulate the "proximity effect", a phenomenon in which a material can become superconducting simply by being placed next to another material that is intrinsically superconducting. This combination can give the two materials new and valuable properties, potentially opening up novel applications in quantum technologies.

The research, carried out in collaboration with the University of Trieste and the California Institute of Technology and published in *Physical Review Research*, has been selected as an *Editors' Suggestion* by the journal. The tool developed in the study could contribute to the development of so-called topological superconductors. These materials are considered key to the realization of topological quantum computers, a new frontier in quantum computing that is attracting major scientific and economic interest. Such a technology would rely on storing and manipulating qubits, the fundamental units of information in quantum computers.
Realistically simulating superconducting interfaces is particularly challenging: the proximity effect can extend over hundreds of nanometres, making conventional computational techniques prohibitively demanding. The new method focuses computational resources on the most relevant region and efficiently combines approaches with different levels of complexity, avoiding the need to explicitly simulate very large structures. In the study, the method was first tested on simplified models and then applied to the interface between $NbSe_2$ and $CrBr_3$, with the results compared against experimental measurements. With this work, the research group provides a technique capable of describing and predicting the proximity effect more accurately, opening up new possibilities for designing and studying combinations of materials and their potential applications, whose properties are still largely unexplored.

From the proximity effect to topological qubits

"When a material is placed next to a superconductor, the former can acquire the same property, as if the two materials were talking to each other," explain Nicolas Baù and Antimo Marrazzo, the first and last authors of the study, respectively. "This is known as the 'proximity effect', a quantum-physics phenomenon with very interesting implications. With our work, we wanted to develop a tool to simulate this physical effect in real materials, with the main goal of understanding how it could contribute to the development of so-called topological superconductors."
Topological superconductors are systems whose definitive experimental realization remains a challenge, but which, according to theoretical predictions, could possess valuable properties thanks to their hypothetical ability to host so-called "Majorana states". "These are special quantum states that could allow quantum information to be stored and manipulated more stably, making quantum computers less vulnerable to errors." This could lead to topological qubits, in which the probability of errors could be drastically reduced thanks to intrinsic protection built into the hardware itself, based precisely on topological superconductors.

A race attracting major interest

The race to develop topological quantum computers is already underway, and some groups have announced devices based on topological qubits. The strength of the evidence supporting these claims, however, remains to be established. “Discovering or creating topological superconductors is by no means easy and, as far as we know, there is currently no definitive proof that they exist,” explain the researchers. Yet there may be a way forward: exploiting the proximity effect. “A conventional superconductor, such as those already used, for example, in magnetic resonance imaging equipment, could produce very interesting results when placed next to another material. The right combination, in fact, could give rise to new and rare properties that neither material possesses on its own, potentially leading to the formation of a ‘hybrid’ topological superconductor. The simulation tool we have developed is aimed precisely in this direction,” the authors explain.

Topological superconductors: searching for the right combination

Reliable computer simulations are essential to pursue this goal. The five authors of the study — Nicolas Baù, Mitra Dowlatabadi, Tommaso Chiarotti, Massimo Capone and Antimo Marrazzo — explain: “These simulations are highly complex because they involve relatively large systems and sophisticated calculations. We have developed a new theoretical framework designed to perform accurate simulations and based on the so-called ‘embedding’ approach: a method that allows the most relevant part of a system to be described in detail, while treating everything else as an effective environment — a ‘bath’ — with which it interacts. “The simulation tool we have developed, which is the subject of this publication, is reliable and realistic because it allows us, on the one hand, to validate what has been done so far and, on the other, to make predictions for real materials, assessing their performance with the goal of identifying genuine topological superconductors. Their potential applications could represent a major breakthrough in the field of quantum computing.”

The significance of the research is further highlighted by its selection as an *Editors’ Suggestion* by the journal, an honour reserved for only around 2% of the papers published by the American Physical Society journal.

The authors conclude: “Our work undoubtedly represents a step forward in this direction. These are predictive and realistic simulations, providing a valuable tool for identifying which combinations of materials may be the most promising and for guiding future experiments towards the realization of topological superconductors based on the proximity effect.

“In the future, we intend to further expand and refine our ‘toolbox’ of computational approaches. At the same time, we will apply these tools to the study of specific combinations of materials, both those already known and those

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that have yet to be explored, also through collaborations with experimental groups such as those at CNR-IOM in Trieste."

LINKS
The paper

IMAGE
Credits: **Nicolas Baù**

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