Simulating strongly correlated fermions opens the door to practical superconductor applications

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This is Boris Svistunov. Credit: Courtesy of UMass Amherst

Combining known factors in a new way, theoretical physicists Boris Svistunov and Nikolai Prokof'ev at the University of Massachusetts Amherst, with three alumni of their group, have solved an intractable 50-year-old problem: How to simulate strongly interacting quantum systems to allow accurate predictions of their properties.

It could open the door to practical superconductor applications, as well as to solving difficult "many-body" problems in high-energy physics, condensed matter and ultra-cold atoms.

The theoretical breakthrough by Prokof'ev and Svistunov at UMass Amherst, with their alumni Kris Van Houcke now at Ghent University, Felix Werner at Ecole Normale Supérieure Paris and Evgeny Kozik at Ecole Polytechnique, is reported in the current issue of *Nature Physics*. The paper also includes crucial results of an experimental validation conducted by Martin Zwierlein and colleagues at MIT.

Svistunov says, "The accompanying experiment is a breakthrough on its own because achieving a few percent accuracy has long been a dream in the field of ultra-cold atoms. We needed this confirmation from Mother Nature."

Van Houcke adds, "Our answers and the experimental results perfectly agree. This is important because in physics you can always make a prediction, but unless it is controlled, with narrow error bars, you're basically just gambling. Our new method makes accurate predictions."

Physicists have long been able to numerically simulate statistical behavior of bosonic systems by mapping them onto polymers in four dimensions, as Richard Feynman proposed in the 1950s. "In a bosonic liquid one typically wants to know at what temperature the superfluid phase transition occurs," Prokof'ev explains, "and mapping onto the polymers yields an essentially exact answer."

But simulating particle behavior in strongly interacting fermionic liquids, like strongly interacting electrons in high-temperature superconducting compounds, has been devilishly elusive, he adds. "The polymer trick does not work here because of the notorious negative-sign problem, a hallmark of fermionic statistics."

Apart from mapping onto the polymers, Feynman proposed yet another solution, in terms of "diagrams" now named after him. These Feynman diagrams are graphical expressions for serial expansion of Green's

functions, a mathematical tool that describes statistical properties of each unique system. Feynman diagrams were never used for making quantitatively accurate predictions for strongly interacting systems because people believed that evaluating and summing all of them was simply impossible, Svistunov points out. But the UMass Amherst team now has found a way to do this.

What they discovered is a trick—called Diagrammatic Monte Carlo—of sampling the Feynman series instead of calculating diagrams one by one. Especially powerful is the Bold Diagrammatic Monte Carlo (BDMC) scheme. This deals with a partially summed Feynman series (Dyson's development) in which the diagrams are constructed not from the bare Green's functions of non-interacting system (usually represented by thin lines), but from the genuine Green's functions of the strongly interacting system being looked for (usually represented by bold lines).

"We poll a series of integrals, and the result is fed back to the series to keep improving our knowledge of the Green's function," says Van Houcke, who developed the BDMC code over the past three years.

The BDMC protocol works a bit like sampling to predict the outcome of an election but with the difference that results of polling are being constantly fed back to the "electorate," Prokof'ev and Svistunov add. "We repeat this with several hundred processors over several days until the solution converges. That is, the Green's function doesn't change anymore. And once you know the Green's function, you know all the basic thermodynamic properties of the system. This has never been done before."

Provided by University of Massachusetts at Amherst

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