

Souping Up Superfluidity Calculations

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“In quantum mechanics, very seldom do you solve exactly problems involving more than one particle,” explains Massimo Boninsegni, Canada Research Chair at the University of Alberta. Boninsegni and his colleagues, Nikolay Prokof’ev and Boris Svistunov, both at the University of Massachusetts, have found a way to work with quantum systems involving many interacting particles on a scale larger than ever attained before. Their creation, named worm algorithm, is a new approach to path integral Monte Carlo (PIMC) simulations, the only known exact general method in quantum mechanics.

Superfluidity is among the most spectacular manifestations regarding the quantum behavior of matter on a macroscopic scale. Superfluids are liquids capable of flowing without resistance, a fascinating phenomenon not yet fully understood. In 2004, another state of particles on the quantum level, supersolids, was discovered. Supersolids act like superfluids (moving without resistance), but maintain the characteristics of crystalline solids.

PIMC is the only known method that can afford the theoretical study of superfluidity, by allowing the simulation, on a computer, of realistic models of superfluids, and by providing exact estimates of key physical quantities, such as the superfluid density. This is where Boninsegni, Prokof’ev, and Svistunov come in. In a letter published in *Physical Review Letters* on February 23, they explain how their worm algorithm overcomes some of the limitations of PIMC, while still making use of its basic ideas.

“If you look at what people were doing by PIMC last year, they were working with the same system sizes as 20 years ago,” Boninsegni tells PhysOrg.com. “It seemed impossible to go bigger. The fundamental approach had to be revisited.” Now, he says, it is possible to have results for systems with 100 times more particles, obtaining more accurate predictions for experimentally measurable quantities such as the superfluid transition temperature. Boninsegni continues, “If it was just about getting more accurate numbers, though, I wouldn’t be so excited. We’ve made it possible to do things that seemed out of reach just a year ago.”

Some of these things include getting a better understanding of defects in solids or the presences of interfaces between two crystalline samples. In order to do that, it is necessary to have a model of a system large enough to show the complex interactions between many particles, and still have particles left over for the interface.

The worm algorithm works by creating entanglement among the particles. This done by “cutting” particles, which Boninsegni explains are “much like strings or polymers that wiggle all over the place.” The polymer-like particles break up and reconnect with other particles in the system. The worm algorithm allows the particle ends to grow and shrink along a fictitious (“imaginary”) timeline. They connect with and disconnect from other particles, but eventually the two loose ends reconnect. By the time the cut polymer finds itself back together, it has created a large permutation cycle. These cycles are crucial to capture the physics of superfluids. The algorithm was originally applied by Prokof’ev and Svistunov to lattice models of space. But a new set of research possibilities (including discovering a possible “superglass” state, in addition to the supersolid state) has emerged from the fact that this particular project has extended the worm algorithm to continuous space, and not just discrete space.

Boninsegni explains that this is not a method of creating a “worm hole,” but rather a mathematical calculation that can better help us understand the underpinnings of our universe. Being able to work with multiple particles and larger, complex systems will open new doors into the possibilities presented by quantum mechanics.

By Miranda Marquit, Copyright 2006 PhysOrg.com

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