Path Integral Monte Carlo Study of Proximity Effects in Confined ^{4}He

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Bridging the Gap Between Theory and Experiment

Performing computational studies of physical systems is crucial because it allows measurements to be made on nanoscale systems that would not be accessible to an experimentalist in a laboratory.

Our group is using Path Integral Monte Carlo (PIMC), an ab initio computational method, to reproduce experimental data gathered by the Low Temperature Research Group at the University of Buffalo, SUNY. They deduced an excess specific heat and an enhanced superfluid response due to the weak coupling of small 'pools' of helium on a Silicon Dioxide wafer. The following shows the superfluid fraction vs. the reduced temperature difference for coupled and decoupled Helium-4.

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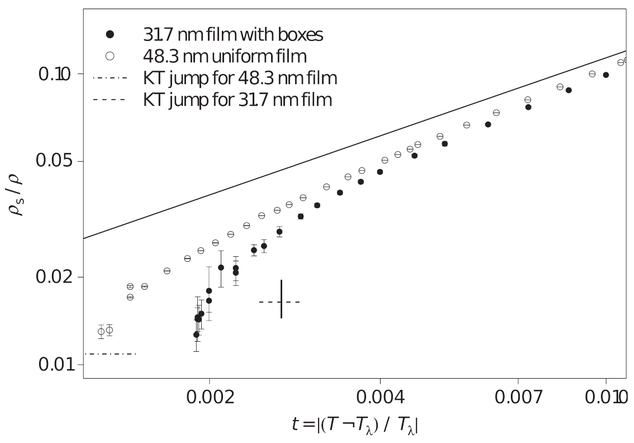

Why PIMC?

PIMC is an exact method, meaning that, given enough computer time, the answers that we obtain from our simulations will be exactly what we would get from an analytic solution! It is based on the path integral formulation of quantum mechanics, via Feynman, and allows the sampling of all possible quantum mechanical paths of a system. This means that the full partition function may be sampled and practically any observable of the system may be measured.

$$\begin{aligned}\mathcal{Z} &= Tr\left[e^{-\beta\mathcal{H}}\right] \\ &= \int D\vec{R}_0 \int D\vec{R}_1 \cdots \int D\vec{R}_{M-1} \left[\langle \vec{R}_0 | e^{-\beta\mathcal{H}/M} | \vec{R}_1 \rangle \right. \\ &\quad \left. \times \langle \vec{R}_1 | e^{-\beta\mathcal{H}/M} | \vec{R}_2 \rangle \cdots \langle \vec{R}_{M-1} | e^{-\beta\mathcal{H}/M} | \vec{R}_0 \rangle \right]\end{aligned}$$

In PIMC, each particle is represented by a closed *worldline* that is made up of a series of positions stepping through imaginary time.

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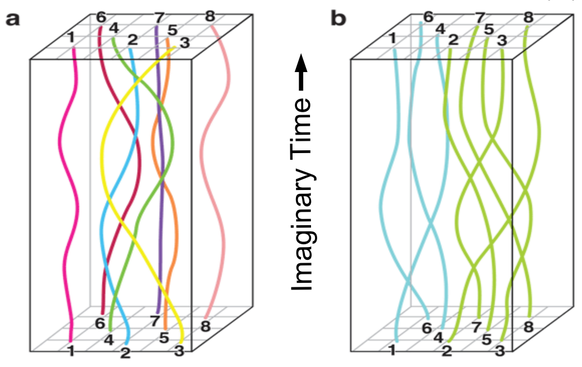
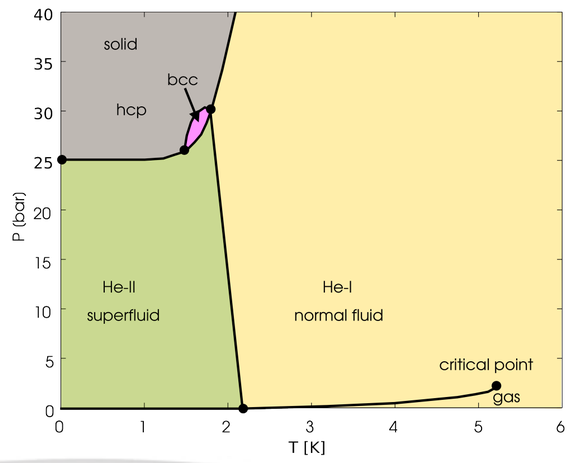


They are periodic in imaginary time, meaning that the final step connects back with the first step. When simulating distinguishable particles (a) , the final step of each worldline must connect with it's own first step. This is not the case for indistinguishable particles (b), as we allow different worldlines to 'mix'. The 'mixing' of these worldlines lead to what is called an *exchange cycle*. This is a distinctively quantum behavior.

Motivation

When Helium-4 is cooled below its critical temperature, an exotic phase of matter is observed which is called a superfluid. This unusual phase is characterized by a non-classical moment of inertia and flow without dissipation. The superfluid phase of ^{4}He is a prime example of macroscopic quantum mechanical behavior. The phase diagram may be seen below.

There is currently no known theory for how thermodynamic properties of a 'dot' of Helium-4 are affected by the coupling of one dot to another, or of how the confinement geometry affects the coupling. The Gasparini Research Group created a SiO_2 wafer with many small wells bored into its surface. This can be seen below.



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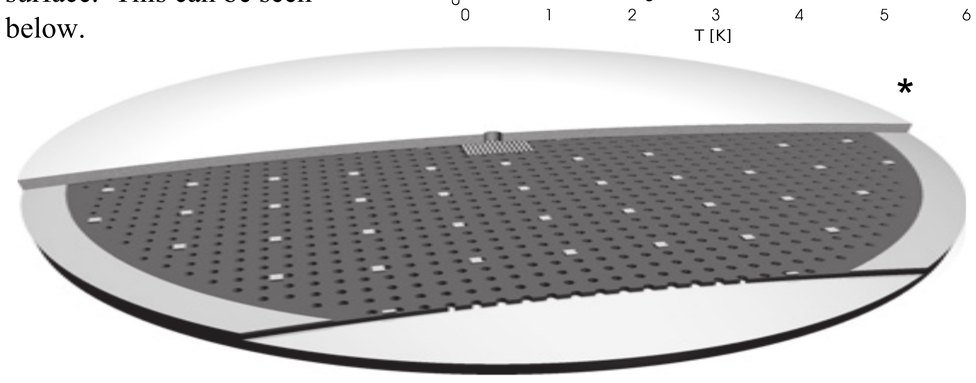
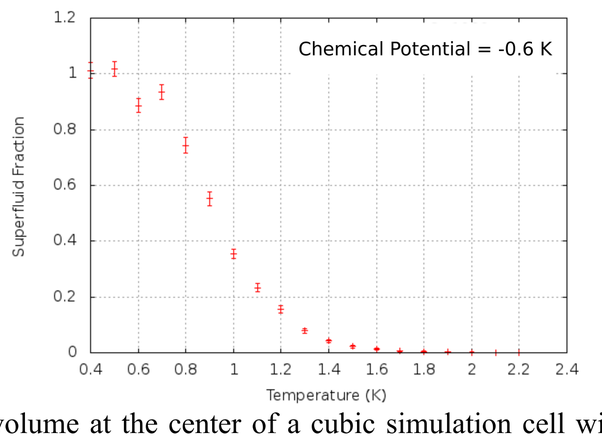


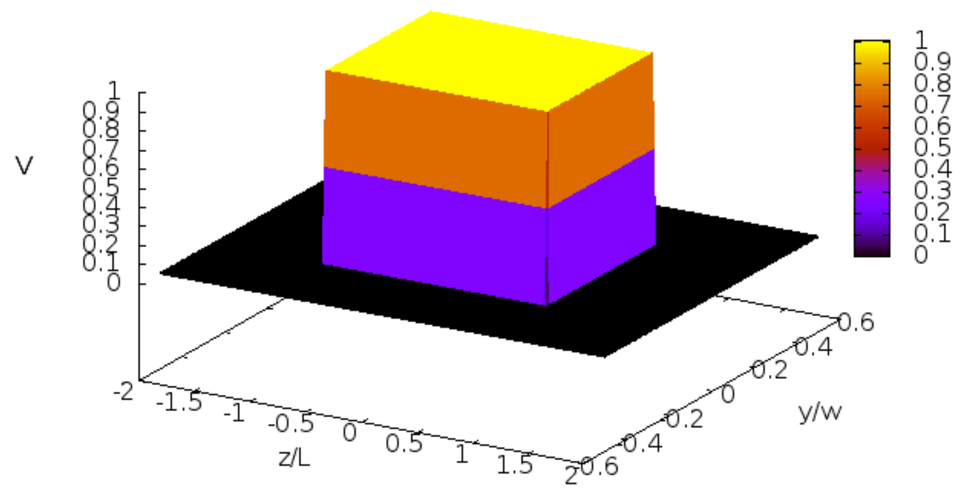
These wells were filled with liquid ^{4}He such that a thin film of Helium was allowed to remain on the surface connecting the wells. Hence, the wells were weakly coupled to one another. We suspect that the enhanced proximity effects are due to the indistinguishable nature of the bosonic ^{4}He atoms. With bosons (quantum mechanical particles with integer spin and symmetric wave functions), the exchange cycles are allowed. This allows for extra degrees of freedom which result in all sorts of exotic behavior such as superfluidity.

Implementation

The film of ^{4}He on the surface of the wafer behaves as a 2-dimensional system. We computed the superfluid transition of ^{4}He in 2-D, as seen below.

The number of atoms we can simulate in a reasonable amount of time using our method is dependent on the computational power available, and is currently but almost any real system will have on the order of 10^{23} atoms. We plan to infer the thermodynamic limit by modeling two weakly coupled dots by excluding volume at the center of a cubic simulation cell with periodic boundary conditions.





We plan to run simulations where we allow the particles to behave as distinguishable and then run simulations where we allow for multi-particle exchange cycles to happen. The different behavior between these two types of simulations is hypothesized to reveal enhanced superfluid response and excess specific heat.

Project Description

There is a great deal to be learned about the quantum mechanical behavior of matter at low temperatures. Recent experimental work has revealed unexplained behavior in confined ^{4}He, and it is our intent to explain this using a method which implements the first principles of quantum mechanics. Due to an innovative take on the PIMC method, our group is one of a handful in the world using a production code capable of providing an answer to this problem. Explaining this phenomenon would shed light on how matter in localized regions of space is affected by weakly connected neighboring regions. Greater understanding of materials which behave quantum mechanically will grant the ability to engineer devices which operate based on the laws of quantum mechanics. Our society will change greatly with the coming of the age of quantum information, and inquiries such as this are necessary if applications are to be realized.

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