Overcoming the Sign Problem in First Principles Calculations

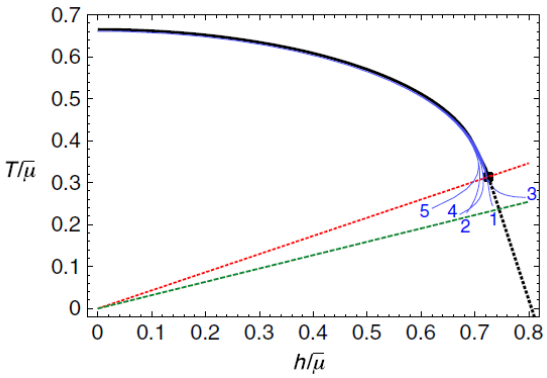

Figure 1- Phase diagram depicting the second order phase transition of an ultracold Fermi gas

A group of physicists have found a method of dealing with the sign problem in *ab initio* calculations involving fermions. They used complex chemical potentials in non-relativistic Fermi gases to solve the sign problem. This technique can be used in many fields including the study of ultracold atoms, condensed matter and quantum chromodynamics.

This sign problem occurs when one numerically evaluates an integral of a highly oscillatory function. Summing up the positive and negative areas of a curve leads to the integral having a very small value. In order to obtain useful information one has to calculate each integral to a high degree of accuracy. According to Dr Joaquin Drut, of the University of North Carolina, dealing with the sign problem is "analogous to trying to extract a small signal from a large amount of noise." This becomes an issue when physicists try to perform first principles calculations involving ultracold fermion gases.

The atoms in the ultracold gases have more spin up particles than spin down. This non-zero polarization creates a sign problem. In order to solve this system, Drut *et al*. proposed a technique involving the use of complex chemical potentials. This is a method used in quantum chromodynamics but was only applied to relativistic particles. They found that using a complex chemical potential eliminated the sign problem but gaining useful information from the simulation proved to be difficult. Running the calculations produced a function which depends on a complex variable. By fitting the curve with another complex function, Drut and his colleagues obtained real valued information. Cases where the curve fitting technique did not work still provided an improvement on previous knowledge. Drut explains that in these cases one can still gain insight into the structure of the partition function in the complex plane. The partition function is useful in the study of phase transitions, including those of ultracold atoms.

Drut *et al.* performed quantum Monte Carlo simulations to show that a tri-critical point is possible for second order phase transitions. This result was achieved using a complex asymmetry parameter in addition to the chemical potential. The asymmetry parameter is found from the difference between the spin up and spin down particles. In order to produce this tri-critical point, an analytic continuation of the potential was required. Drut notes that this is not always possible, however "Even in cases where the continuation is not valid, you can still find non trivial information. This is crucial because before we had nothing."

The use of complex chemical potentials is a technique that can be used to resolve the sign problem in quantum Monte Carlo simulations. This method has the potential for a broad impact in many branches of physics. It is particularly interesting in when trying to model ultracold fermion gases due to the accuracy of experiments according to Drut. He says, "It also has a very versatile application in ultracold

atoms. Experimentalists in this field can fine tune their systems which gives us a great opportunity to check our methods." Drut and his colleagues are currently developing ab initio code with complex chemical potential functionality. This code will be tested rigorously and compared to experiment. When it is released it will be a great tool for many theoretical physicists especially those in condensed matter and atomic physics.

Summary for use in RSS feeds

The use of complex chemical potentials was shown to be an effective method in overcoming the sign problem in quantum Monte Carlo simulations. It is particularly useful in the study of non-relativistic particles and can be used to generate phase diagrams. The results obtained have applications in the fields of quantum chromodynamics, condensed matter and atomic physics.

Interview Transcript

Q: What were the motivations for tackling this problem?

A: There were many motivations that drew us to this problem. There are in nature a lot of problems that cannot be treated with paper and pencil methods. You know from your studies in quantum mechanics that you can solve a few problems analytically. However when you start to add more than two particles then it becomes very difficult to treat. But there is a many body aspect to these problems in nature that makes them difficult to solve without computers. Quantum chromodynamics is one of those problems in addition to condensed matter and quantum chemistry. You might think that "why don't you just put them in a computer?" That sounds easy and all you would need is an expert programmer. This problem however is not trivial. One of the complications that arises is the sign problem.

Q: What is this sign problem that comes up in these numerical simulations?

A: The sign problem appears in situations often in situations that aren't related to quantum mechanics. It comes up when you need to evaluate an integrand that is highly oscillatory. This means that when you do the integral the number is very small but if you did it for the absolute value it would be huge. It's analogous to trying to extract a small signal from a large amount of noise. You can also regard it in the same way that people have been searching for the Higgs boson in the sense that there are a lot of particles to sort through. There have been studies in a generic way that concluded the sign problem is what is called an np problem. This means it is a very hard problems that is difficult to solve with computers and you would require an exponential amount of time.

Q: If the problem is exponentially difficult, how did you solve it?

A: In this particular case that we treated, we had a system of non-relativistic particles. This could be ultracold atoms which people study in labs all over the world. If you want to study those systems with computers, you run into a problem in which you have more particles with spin up than spin down. When you have a non-vanishing polarization then you run into a sign problem. You have an integrand that is highly oscillatory. We proposed that if you do the integral with complex variables instead of real ones. In

this case you can analytically continue along the real axis. This was a strategy that was applied in quantum chromodynamics but was never applied to our particular problem.

Q: Does this method look like it will be a useful tool in getting rid of the sign problem?

A: If you do this with a chemical potential, you do not actually have a sign problem. Now the question becomes can you extract useful information from these types of calculations. We concluded that you can and you can perform numerical studies to see what you can get from these calculations. We do not solve all the sign problems but it is at least a step forward. One case where this does not work is when the interaction is repulsive. However if the interaction is attractive then we are fine and we can treat the polarized case with these complex potentials. After we obtain the numerical results, we can see what we can extract in terms of going to the real axis. From that we can obtain some real physical information.

Q: Is it as simple as taking the real part of the answers? Or does it involve the projection onto the real axis?

A: It is similar to that, however it is a bit more complicated. What you need to do is extract a whole function that will be a function of some variable. You then need to fit that curve with a function that is dependent on another imaginary variable. Eventually the i cancels the i and you get a real value. If the analytic continuation is valid then you can get useful information. Even in cases where the continuation is not valid, you can still find non trivial information. This is crucial because before we had nothing.

Q: What sort of information can you expect if the continuation is not valid?

A: The analytic properties of this partition function are very useful in phase transitions. Even when you can't get information about the real axis, it is still good to know the structure of Z in the complex plane.

Q: Sort of as an aside, what kind of response has there been to this new technique?

A: We received a very good response when it was presented in Germany a couple of months ago. We also had a great response from the referees when this paper was published. It was well understood that this paper could have broad impacts. It is a technique used in quantum chromodynamics but now it is brought to the attention of atomic physicists and condensed matter theorists. And it allows the chromodynamics people to study a problem that is quite simple and better understand the technique. It also has a very versatile application in ultracold atoms. Experimentalists in this field can fine tune their systems which gives us a great opportunity to check our methods.

Q: Have there been updated ab initio codes with this functionality built in? Are you in the process of developing them?

A: We are in the process of making these codes by building it into existing code. The hard part is testing the code since no one had run these types of simulations before. Once our code is well tested and the results are published on the arxiv then we will make our code available.

Q: Thanks again for doing this and best of luck with the code development!

A: No problem! Thanks for taking an interest in my work!