New computational tools for the modelling of correlations in quantum systems.

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December 16, 2010

The Quantum world exhibits phenomena that sometimes appear counterintuitive. Superconductivity is a well known example. To understand the quantum world, we have to resort to mathematical models that lead to complicated mathematical equations. Often approximate solutions to these equations are sufficient to describe quantum phenomena, as is seen for example in the Bardeen-Cooper-Schrieffer (BCS) mean field theory of superconductivity. If one wants to study more complicated quantum correlations, one has to rely on methods that go beyond the mean field. The Richardson-Gaudin (RG) models offer a promising approach in this respect, because they describe the quantum correlations in superconductors while the corresponding mathematical equations can be solved exactly. Although easily written down, actually solving the RG equation for more than a few particles turns out to be a cumbersome task due to singularities that occur in the resulting mathematical equations. The fact that standard non-linear solver techniques can not handle these singularities has made that the RG models have yet failed to attract all the attention they deserve.

One of the important breakthroughs of the Quantum Modelling project was the development of a computer code that can solve the RG equations efficiently even for thousands of particles. This opened the way to extend the use of RG models as a fundamental tool to analyze correlations in quantum systems. In particular, we investigated three situations where BCS theory fails to give the complete answer: ultrasmall metallic grains [1], atomic nuclei [2] and p-wave superconductors [3].

Ultrasmall metallic grains offer a different perspective on superconductivity: their limited size hinders the formation of quantum correlations, which raises the question up to what size one can identify them as superconductors. RG models allowed to analyze quantum correlations in grains as a function of size, showing that the pair correlations characteristic of superconductivity can persist at ultrasmall sizes, even though they might not manifest superconductivity in the traditional sense.

The RG equations describe quantum correlations under the idealistic condition of zero absolute temperature. To include the effect of finite temperature, while maintaining the exact quantum correlations, we used the Quantum Monte Carlo method (QMC). This method is based on a statistical sample of quantum configurations, such that one obtains statistical estimates of physical quantities. The important point here is that for the RG models one can generate *unbiased* samples. Then, using modern day parallel computer clusters, one can generate sufficiently large samples to obtain the exact result with negligible statistical error.

The RG models also describe pair correlations in atomic nuclei. These correlations have a profound influence on the nuclear level densities, an important ingredient to calculate the nuclear reaction rates that govern astrophysical processes in neutronstars and supernovae. Using the RG model together with the QMC method, we were able for the first time to calculate how pair correlations affect the nuclear level density while at the same time maintaining the exact rotational symmetry.

Finally, a lot of effort went into the study degenerate Fermi gases. The constituents may be neutral atoms, as is the case in trapped Fermi gases of ^{40}K and ^{6}Li or superfluid ^{3}He, or charged electrons as in conventional metallic superconductors, nucleons in heavy nuclei or nuclear matter. The particular nature and symmetry of the interactions may lead to exotic superfluid phases with complex order parameters, as is well-known in the case of liquid ^{3}He.

We focused on an order parameter with p-wave symmetry that might be encountered in ultracold Fermi gases or in exotic superconductors such as Sr_2RuO_4. The spinless RG model with $p_x + ip_y$ pairing interaction provides a schematic model that captures the basic physics of the Bose-Einstein Condensate and BCS superfluid sides of the phase diagram. The exact solution of the model offers detailed insights into the phase transition mechanism.

Even though the $p_x + ip_y$ model has been studied before, we reach drastically different conclusions about the zero temperature quantum phase diagram. Our numerical and analytical results show that the quantum phase diagram exhibits a third-order quantum phase transition when the chemical potential changes sign. This transition is characterized by a logarithmically diverging length scale that can be obtained experimentally from correlations in the density fluctuations. Thus, in a certain sense, our physical picture is that the strong-pairing region represents a confined superfluid phase while the weak-pairing region is the deconfined phase.

We show that these are general features of the hyperbolic RG model, irrespective of the specific symmetry or dimensionality of the representation. This means that our conclusions equally apply to other models that can be derived from the same RG equations, be it models for pairing in atomic nuclei, or Jaynes-Cummings like models of resonantly coupled fermionic atoms.

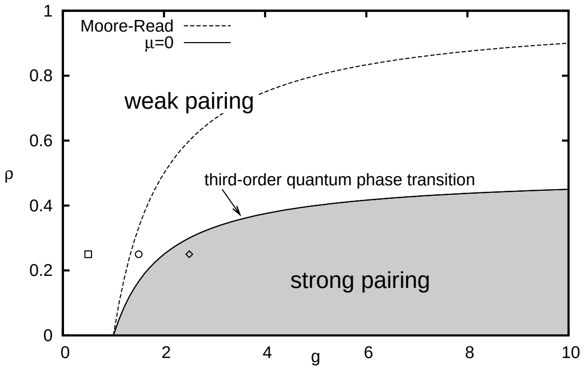

Figure 1: Quantum phase diagram of the $p_x + ip_y$ or hyperbolic RG model in terms of the fermion density ρ and the attractive coupling strength g. It shows two superfluid phases, a strong-pairing (confined) and a weak-pairing (deconfined) phase, separated by a third-order confinement-deconfinement QPT at vanishing chemical potential.

To maximize the scientific impact of the Quantum Modelling project, an effort is underway to release our computer code for the RG equations under an open source license, such that the RG models can become a new computational tool wherever they can provide insights that can not be obtained from established quantum many-body techniques.

References

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