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Solution to the sign problem in a frustrated quantum impurity model

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ABSTRACT

In this work we solve the sign problem of a frustrated quantum impurity model consisting of three quantum spin-half chains interacting through an anti-ferromagnetic Heisenberg interaction at one end. We first map the model into a repulsive Hubbard model of spin-half fermions hopping on three independent one dimensional chains that interact through a triangular hopping at one end. We then convert the fermion model into an inhomogeneous one dimensional model and express the partition function as a weighted sum over fermion worldline configurations. By imposing a pairing of fermion worldlines in half the space we show that all negative weight configurations can be eliminated. This pairing naturally leads to the original frustrated quantum spin model at half filling and thus solves its sign problem.

1. Introduction

Understanding quantum many body physics, especially in the regime where the degrees of freedom are strongly correlated, is one of the outstanding areas of research in both condensed matter and nuclear physics today. Many physical phenomena ranging from the properties of nuclei [1], phases of dense nuclear matter [2], properties of high T_c materials [3], heavy fermion systems [4], topological superconductors and insulators [5], etc., contain strongly correlated regimes of interest.

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While approximate methods can help uncover exotic features that can emerge in such systems, reliable quantitative predictions usually require numerical approaches such as the quantum Monte Carlo method [6–11]. Unfortunately these methods suffer from sign problems in many interesting cases, and their solutions are exciting research directions in the field of computational quantum many body theory today [12].

The challenge is to rewrite the quantum problem as a classical statistical mechanics problem with positive Boltzmann weights that are computable in polynomial time. While the Feynman path integral is one way to proceed, the presence of fermions and/or frustration means there is no guarantee that the goal can be achieved. Although a generic solution that solves all sign problems most likely does not exist [13], solutions to specific sign problems can be found and there is a long history of such solutions for problems in thermal equilibrium. These fall under three broad categories: (1) Finding the right basis for the Hilbert space such that sign problems are absent, (2) finding a resummation of the partition function that renders the resummed weights positive, and (3) finding a symmetry such that every term of the sum can be written as a square of real number. Examples of the first category include anti-ferromagnets on bi-partite lattices and solutions to a class of frustrated quantum spin systems [14,15]. The second category includes methods like the meron-cluster method [16,17], the subset method [18–20] and the fermion bag approach [21–23]. Solutions to fermion sign problems can be obtained by combining ideas from (2) and (3) [6–8,10,9,11]. Recently ideas from all the three categories have been combined, especially with the use of perturbative diagrammatic expansions of the partition function [24–26], to solve new sign problems [27–34]. In contrast to systems in thermal equilibrium, sign problems also arise when solving real time dynamics of quantum problems. Recently, some progress has also been made in solving these more difficult sign problems [35–38].

Although many solutions to sign problems exist, frustrated quantum systems continue to be the most challenging among problems in thermal equilibrium. Recently, it was shown that sign problems in a class of frustrated quantum spin systems when formulated in the local spin-half basis can be eliminated by going to a local spin-one basis [14,15]. A natural question is whether this approach is helpful to solve other types of frustrations not considered so far. In this work we discover a solution to a simple frustrated model involving a single triangular anti-ferromagnetic interaction. In order to make the problem non-trivial, each spin in the triangle is coupled to its own bath of spins in the form of a one-dimensional chain. This model contains a geometrically different type of frustration than those considered in [14,15]. However, our final solution is similar and emerges when the system is formulated in a local spin-one basis on half the system. Interestingly, we can go a step further and show that the solution is based on fermion pairing in a related fermion model. It would be exciting if a systematic approach could be developed to construct the correct basis that solves the sign problem for every problem of interest. We believe our work takes us a step closer towards this goal. Our model was considered earlier as a toy model to explore if a basis change could help alleviate the sign problem [39]. It was shown that even a small change in the basis can have a significant effect on alleviating the sign problem. In this work we show that the sign problem can in fact be completely eliminated.

Our paper is organized as follows. In Section 2 we explain the details of our model and map it into a fermion model which plays an important role in uncovering our solution. In Section 3 we transform the model into an inhomogeneous one dimensional model by identifying new fermion degrees of freedom on half the lattice. We then expand the partition function using fermion worldlines and identify the origin of the sign problem. In Section 4 we show that the sign problem is absent in a model that contains only paired fermion worldlines. Using this insight, in Section 5 we define a new local basis for the original spin model that is free of sign problems. Section 6 contains our conclusions.

2. Frustrated quantum impurity model

In this work we consider a model consisting of three quantum spin chains constructed with spin half operators $\mathbf{S}_{a,i}$, where $a = 1, 2, 3$ labels the three chains and $i = 0, \ldots, N$ labels the sites in each chain. Frustration is introduced through an anti-ferromagnetic interaction among the three quantum