RESEARCH ON DENSITY MATRIX RENORMALIZATION GROUP CALCULATION OF TWO-CHANNEL KONDO MODEL

The Kondo problem has been a hot research topic in physics since the 1960s. This type of quantum impurity model refers to the interaction between magnetic impurities at low-dimensional quantum dots and the high-dimensional external environment. For example, the Kondo effect refers to conduction electrons exhibiting only a slight antiferromagnetic effect near the impurities at higher temperatures, and in contrast, as the temperature approaches zero, the impurity magnetic moment and a conduction electron magnetic moment strongly combine to form an overall nonmagnetic state. Moreover, there is a Kondo resonance effect, which is reflected in the presence of several periodic sharp peaks in conductivity at low temperatures.

The Hamiltonian of the two-channel Kondo model is as follows:

$$H = -t \sum_{i(chain1,chain2)\sigma} \left(c_{i\sigma}^{+} c_{i+1\sigma} + h.c\right) + J \sum_{i(chain1,chain2)} S \cdot s_i \tag{1}$$

Two-channel Kondo model has various interesting physics,. For example, at the early stage of research people found that even at zero temperature, the model would have a finite entropy, corresponding to additional degrees of freedom. Later, this effect was found to be a result of the Majorana fermion .What conduction electrons couple is no longer a single impurity operator, but the sum of production and annihilation operators. This is also the definition of the Majorana operator. The two-channel Kondo model does not only exist in theory and simulation, its existence and physical properties have been confirmed by experiments. More physics comes from the two-channel kondo effect coupling with other interactions. For instance, when considering actual one-dimensional chains, interactions between multiple quantum dot impurities, such as the RKKY spin-orbit coupling mechanism, may destroy the original Majorana structure.

I'm going to calculate the properties of entanglement in a two-channel Kondo model. There' s article using the analytical results of conformal field theory to derive the form on the entanglement of the two-channel Kondo model. What is simulated is the relationship between entanglement entropy and the system size. That is, several grid points in the middle of the system including local spin are selected as subsystems to calculate the entanglement entropy. By changing the size of the subsystem, from only containing local spins to the entire two-channel Kondo model, the entanglement between the two subsystems is calculated as the size of the subsystem changes, which reflects the structure of the entanglement entropy. I will observe the change of entanglement entropy by changing the value of kondo interaction, which can determine the nature of the phase transition and help master more physics of the two-channel Kondo model.

The method I use is the density matrix renormalization group (DMRG) method. The Numerical Renormalization Group (NRG) algorithm was proposed by Wilson in the 1970s to solve the low-energy physical properties of the spin chain model. By applying the renormalization group ideas, the NRG eliminates some high-energy parts in the Hamiltonian matrix, while retaining the dimensions of the low-energy parts. During such repeated operations, the energy will converge, and the obtained fixed point is the ground state energy. Later, White introduced the DMRG approach to solve the large errors of NRG when introducing lattice interactions or selecting specific boundary conditions. The idea of DMRG is that since the sum of the density matrix eigenvalues is one, the value of k can be chosen cleverly so that the sum of the first k eigenvalues is close to one, and there will always be some states close to zero. This situation occurs frequently in condensed matter physics, especially in systems at zero temperature. In the case where the ground state is non-degenerate, some eigenvalues of the density matrix may be zero, corresponding to pure states of the ground state. To conclude , DMRG cutoff density matrix instead of Hamiltonian matrix to decrease the error. The basic approach of DMRG also uses the idea of renormalization, analogous to the method of intercepting the Hamiltonian matrix, we still start from a small number of grid points, expand the Hamiltonian by adding points, and obtain the ground state energy and eigenvalues after diagonalization to construct a density matrix Then do the truncation and repeat the process. In addition, for a one-dimensional finite system, if only one system block is selected as the growth block, the physical effects brought by the remaining parts will be ignored, and there will not be enough iterations during the growth process. Instead, the system should be divided into two blocks: system and environment, and growth should be done separately. When forming the Hamiltonian matrix, it is necessary to combine two blocks to form a super block, perform diagonalization, and obtain the density matrix of the super block, thereby obtaining the reduced density matrix of the system block, truncate the reduced density matrix, and then grow the system block and environment block, repeat the above process and we will have the ground state energy for infinite systems. The approach for finite systems is similar after considering sweeps of the two blocks. The entanglement entropy plays an important role in the error of the DMRG approach. The core idea of the DMRG approach is to reduce the degrees of freedom of the system by retaining the most important entanglements in the system, thereby reducing the computational complexity. If the entanglement of the system does decay very quickly with respect to the dimension number of the matrix, then the error caused by truncation will be very small.

Matrix Product States (MPS) are a state representation method used to describe quantum many-body systems. Matrix product states are constructed through the product of a series of tensors, each tensor corresponding to a degree of freedom in the system, and describe the entangled structure of the quantum state through specific constraints. By limiting the entanglement index and utilizing the orthogonality of tensors, matrix product states can effectively describe the entangled structure of quantum many-body systems and provide a compact representation. For processing larger lattice system matrix product states, the tensor is stored in the operation instead of the state vector, which can reduce the complexity of the storage in the operation. This study is based on the use of the Itensor program (https://www.itensor.org/). The Itensor package provides a method for constructing matrix product states. It uses the fast representation of tensor networks to quickly express the role of the Hamiltonian on the matrix product state, thereby solving key physical quantities such as ground state energy and entanglement entropy.

Before using Itensor package to of the 2CK problem, I start from considering a limited number of particles to find an analytical solution. Specifically, I used two methods to solve it. The first is to use extreme cases to solve. I considered the situation where the Kondo interaction parameter J is equal to zero or the conduction electron transition parameter t is equal to zero. Secondly, I also used the Exact Diagonalization (ED) package Quspin. This method can obtain accurate results by accurately calculating the eigenstates and eigenvalues of the system .Following the ED approach, the eigenvalue of the reduced density matrix is calculated. For example, solving the Hamiltonian matrix at 8 dimensions, when J=1,t=0, the value of entanglement entropy for three sites is 0.636514. The same result can be obtained by using the DMRG program in the appendix to substitute the total number of grid points as three, ignoring the coupling between electrons, and setting the Kondo interaction parameter to J=1.

Next I used the Itensor package. The DMRG program used in this study relies on the Itensor tensor calculation package, using the Intel Mkl math library. The first program running platform is the local Windows wsl2 virtual environment; the second is the Siyuan No. 1 supercomputing platform of Shanghai Jiao Tong University. The calculation results of this article have received support and help from the High Performance Computing Center of Shanghai Jiao Tong University. The initial state may play a role in the calculation. This initial state needs to satisfy some restrictions on orthogonal basis parameters. In order to comply with the laws of physics, we chose the initial state with the total spin of the conduction electron being zero. In this case, I chose the half-filled orthogonal basis as the initial state. If we look at the Hamiltonian matrix composed of an orthogonal basis without any parameter restrictions, we see that the Hamiltonian can be partitioned according to different total number of particles. This shows that choosing different total particle numbers has a huge impact on the ground state energy. There are two main reasons why this is a reasonable choice when the system is half-filled. First, the half-filled state has completely symmetrical properties, which makes calculations much simpler. Secondly, the half-filled state has rich properties in physics, among which the Neel state is a common choice.

By applying the density matrix renormalization group (DMRG) method to calculate the two-channel Kondo model, we obtain the relationship between the ground state Kondo partial energy and the entanglement entropy as a function of Kondo interaction strength. Preliminary results show that the ground state energy of the Kondo part shows a decreasing trend, which may be approximately a linear relationship. At the same time, when the Kondo interaction strength J approaches the limit, the entanglement entropy tends to be saturated, and there is an asymptote. When J is small, the entanglement entropy gradually increases from zero, but it does not complete it all at once, but goes through multiple entanglement entropy platforms.

Considering the Asymptotic behavior of entanglement entropy. The rising pattern of entanglement entropy is that as the Kondo interaction increases, the entanglement entropy rises rapidly and reaches saturation, corresponding to the Kondo singlet state, of which the entanglement entropy is ln2 ,just as the kondo singlet predicts. Then the entanglement entropy will slowly change, and at this time the phase transition is approaching the end. The approximate position corresponding to the end of the rising period is around J/t=2.2, indicating that a phase transition from the antiferromagnetic Neel state to the Kondo singlet state occurred in this interval of 0 to 2.2.

Considering the effect of system size, it was found that when the system size is small, the entanglement entropy will appear a ”platform”. When the system size approaches the thermodynamic limit, this platform gradually disappears and the entanglement entropy rises smoothly, which is result of finite size effect. Under the thermodynamic limit, a large number of eigenstates correspond to energies near the ground state, but due to different spin arrangements, they correspond to different entanglement entropies. The ground state changes continuously among these states as the Kondo interaction increases. Since the ground state is also formed by the degeneracy of a large number of these states, the corresponding entanglement entropy of the ground state also changes continuously. In the case of finite grid points, as the Kondo interaction increases, the ground state changes discretely in these states. Corresponding to a certain Kondo interaction interval, a certain type of spin arrangement mode may be dominant, and the corresponding ground state entanglement entropy also changes discretely., embodied in these ”platforms”.

Considering the effect of boundary condition, the rising behavior of the entanglement entropy of the periodic boundary condition of the two-channel Kondo model is the smoothest, and the entanglement entropy of the periodic boundary condition of the double-channel or single-channel model rises more smoothly than that of the open boundary condition. The periodic boundary conditions ensure the discrete translational symmetry of the system, allowing the head and tail electrons to conduct each other, which actually weakens the finite size effect of the system, making the system’s entanglement entropy rise most smoothly under periodic boundary conditions. Considering the distribution of entanglement。I calculated negativity。There is no symmetry breaking during the phase transition in the two-channel Kondo model, and the entanglement distribution between the two chains is uniform. Regarding the distribution of entanglement, both the distribution of Kondo energy in the left and right channels and the negativity of entanglement between the two channels are consistent in the stable phase. This is actually consistent with physical reality and indicates that the partial transposition process does not introduce new singular eigenvalues, and all entanglement can be described by entanglement entropy. The entanglement brought by entanglement entropy is the main form of entanglement between the local spins and other parts of the system. It is not appropriate to discuss the two chains separately because it will not introduce new singular entanglement.

To conclude, the two-channel Kondo model has unique ground state and entangled properties. Through research on the density matrix renormalization group algorithm, I successfully constructed a matrix product operator and a matrix product state composed of tensor network states, and used the density matrix renormalization group algorithm to process one-dimensional two-channel Kondo The entangled nature of the model. I first used analytical methods to obtain the ground state and entanglement entropy of the two-channel Kondo model under a small number of lattice points, thus verifying the correctness of the density matrix renormalization group algorithm I wrote. Then apply the program to different parameters J/t, different system sizes, and different boundary conditions to obtain the properties of entanglement entropy. I think that the asymptotic behavior of entanglement entropy corresponds to Kondo singlets, the platform of entanglement entropy corresponds to the finite size effect, the results of applying periodic boundary conditions are better than open boundary conditions and the distribution of entanglement between two chains.