The t-J model

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1 Introduction

The t-J model is a way to describe high critical temperature (T_c) super conductivity. The model has been around for decades, but interest has varied. The t-J model describes strongly correlated electrons on a lattice, but does not allow two electrons on one lattice-site. It is a simple model, but powerful enough to capture the interesting physics of high temperature superconductivity and cuprates.
There is interest in finding a general solution for the ground state in one dimension (1D), as in [1], but no solution for general values of J/t has been found yet, although there have been solutions found for specific values of J/t using the Bethe-ansatz. In the t-J model, t determines the strength of the hopping-term, where J is the strength of the interaction term, either repulsive or attractive.

The 2D case is even much more complex, but it is also more interesting due to the formation of Cuperates. There have been attempts to solve the t-J model in 2D using Quantum Monte Carlo Simulations (QMCS). [2] Recently, also machine learning methods like artificial neural networks, have been used and yield interesting results. [3] Given the well known fermion sign-problem in using numerical calcuations for fermionic spin-lattice models, these methods give solutions with exponentially large errors, and therefore are not definite.

Here I attempted to use ALPS, an implementation to simulate different spin-lattice models in Python.
Besides the 'classical' interest from the condensed matter physics community in solving the t-J model once and for all, there could be applications of the t-J model in other fields. For example the Ising model has been used to describe collective behavior like swarming in flocking in biophysics. [4]

2 Model & Methods

2.1 The t-J model

The t-J model describes strongly correlated electrons on a lattice in d dimensions. The repulsive interactions between the electrons prevents them from occupying a site together, thus there can only be one or zero fermions on a single site. The particles can still be in two different states, spin-up or -down. ([5]) The t-J model, equation 2 ([1]), is derived from the Hubbard model, equation 1 ([6]), by taking the strong coupling limit ($U/t >> 1$). Therefore, $J << t$ in the resulting t-J model derived from the Hubbard model, in general this is not a requirement for the t-J model. Therefore the t-J model needs to be solved individually and we can not just use the solutions for the Hubbard model by taking the strong coupling limit of these solutions.

Supersymmetry (SU(2) symmetry) in the t-J model is best explained by the fact that no two fermions are allowed at one lattice-site. So adding a spin-up fermion to site i, means that if there is a spin-down fermion at site i, it needs to be annihiliated. The same is true for holes, if there is a hole at site j, then adding a up- or down-spin fermion means the hole is annihiliated. [7]

$$H^{Hubbard} = \sum_{<i,j>} t c^{\dagger}_{i,\sigma} c_{i,\sigma} + \frac{U}{2} \sum_{i,\sigma} n_{i,\sigma} \sigma_{i,-\sigma} \tag{1}$$

$$H^{t-J} = t \sum_{<i,j>} (X^{\sigma,0}_j X^{0,\sigma}_i + X^{\sigma,0}_i X^{0,\sigma}_j) + J \sum_{<i,j>} (S_i \cdot S_j - \frac{1}{4} n_i n_j) \tag{2}$$

The formulation of the Hamiltonian used here is the one used by Sarkar in [1]. Here $X^{0,\sigma}_i$ is an operator that destroys an electron with spin $S_z = \sigma$ at site i and leaves a hole. The exchange interaction is given by J, wich is $J = \frac{2t^2}{U}$. The second term in the Hamiltonian is exactly the anti-ferromagnetic Heisenberg model, this term describes the exchange interaction between spins. It gives a first insight to why this model can be used to describe superconductivity.

2.1.1 1D and the Bethe ansatz

As mentioned before, the t-J model can be solved exactly in one dimension using the Bethe ansatz, as showed in [1]. However, the solutions depend on the value of $\frac{t}{J}$. Here we will look at solutions for the case where we have a lattice with N sites, containing (N-2) up-spin fermions ($\uparrow$), one down-spin fermion ($\downarrow$) and one hole (0). The solutions differ for different values of t/J, which means that the solution is dependent on the separation between the up-spin and the hole.

Before imposing the Bethe ansatz, the SU(2) algebra can be extended to the U(1/2) superalgebra. For this a harmonic oscillator representation is introduced. (3) Here b creates a hole, whereas f_i^σ annihiliates a fermion at site i. Remember that the t-J model prohibits two fermions to occupy one site, even when these fermions are in different states, but every site is occupied, since hole states are not equal to vacuum states. This means that there are no longer four different states for a site; $|\uparrow\downarrow\rangle, |\uparrow\rangle, |\downarrow\rangle, |0\rangle$, since double-occupied states are not possible anymore. We are left with the following states; $|\uparrow\rangle, |\downarrow\rangle, |0\rangle$.

$$X^{0\sigma} = f^\sigma b^\dagger X^{\sigma 0} = b f^{\sigma\dagger} \tag{3}$$

Now, rewriting the Hamiltonian in 2, we get equation 4 where $P_{i,i+1}$ is a permutation operator, which is defined in 5. In equation 5 the σs are the Pauli matrices.

$$H = \sum_i t(b_i f_i^{\sigma\dagger} f_{i+1}^\sigma b_{i+1}^\dagger + b_{i+1} f_{i+1}^{\sigma\dagger} f_i^\sigma b_i^\dagger) + \frac{J}{2}(P_{i,i+1} - 1) \tag{4}$$

$$P_{i,i+1} = \frac{1}{2}(\sigma_i \cdot \sigma_{i+1} + 1) \tag{5}$$

The permutation operator works as shown in equation 6; it exchanges the creation operators of site i with the one for site $i+1$.

$$P_{i,i+1}(...f_i^{\alpha\dagger} f_{i+1}^{\beta\dagger} |0\rangle) = ...f_i^{\beta\dagger} f_{i+1}^{\alpha\dagger} |0\rangle \tag{6}$$

For the described N-site lattice the state is expressed as below (7). Where x_1 is the position of the up-spin fermion and x_2 is the location of the hole.

$$|\psi\rangle = \sum_{x_1,x_2} f_1^{\uparrow\dagger} f_2^{\uparrow\dagger} ... f_{x_1-1}^{\uparrow\dagger} f_{x_1}^{\downarrow\dagger} f_{x_1+1}^{\uparrow\dagger} ... b_{x_2}^\dagger ... f_N^{\uparrow\dagger} |0\rangle \tag{7}$$

$$H|\psi\rangle = E|\psi\rangle \tag{8}$$

The Schrodinger equation (8) can't be solved in the most general way for the t-J model, so first the results for the simplest case will be shown. This is the scenario where x_1 and x_2 are far apart.
Using the Schrodinger equation as in Eq. 8and filling in a general, yet undetermined function α we get Eq. 9.

$$E\alpha(x_1,x_2) = -J\alpha(x_1,x_2) + \frac{1}{2}J[\alpha(x_1+1,x_2)+\alpha(x_1-1,x_2)] + t(\alpha(x_1,x_2-1)+\alpha(x_1,x_2+1)) \tag{9}$$

Now substitute in the general Bethe ansatz for α given by:

$$\alpha(x_1, x_2) = \sum_{P,Q \in S_2} A_P(Q) \exp\left(i \sum_{j=1}^{2} k_{P_j} x_{a_j} \right) \theta(x_Q) \tag{10}$$

Where $\theta(x_Q)$ defines the sector where $x_{Q_1} < x_{Q_2}$. P, Q are permutations belonging to the group S_2, k_j are quasi-momenta, that are undetermined at the moment and the A_p are coefficients.

Filling the Bethe ansatz (10) into the Schrodinger equation for the t-J model (9) results in:

$$E(A_1(1)\exp(i(k_1x_1 + k_2x_2)) + A_2(1)\exp(i(k_2x_2 + k_1x_2))) = 2(\frac{1}{2}J\cos(k_1) + t\cos(k_2))A_1(1)\exp(i(k_1x_1 + k_2x_2)) \tag{11}$$

In equation 11 shorthand notation is used,

$$Q = 1 = \begin{bmatrix} 1 & 2 \\ 1 & 2 \end{bmatrix}$$

and $Q = 2 = \begin{bmatrix} 1 & 2 \\ 2 & 1 \end{bmatrix}$ and similar for P.

The solution found here only holds for $|\frac{J}{2t}| = 1$ due to the conditions on the Bethe ansatz.

The second situation that is solvable is when x_1 and x_2 are nearest-neighbors. Solving the Schrodinger equation for this situation results in the conditions on the coefficients A as in equation 12.

$$A_1(1) = u^{12}A_2(1) + v^{12}A_2(2) \text{ and } A_1(2) = u^{12}A_2(2) + v^{12}A_2(1) \tag{12}$$

it is found $|t/2J| = 1$. It is needed that $u(k_1, k_2)v(k_1, k_2) + v(k_2, k_1)u(k_2, k_1) = 0$. This condition fails, which leads to the solution of using the permutation operators P_L, the difference between P_L and P is found in the fermionic nature of the operators f^σ, although the difference between bosons and fermions in one-dimension is different from that in higher dimensions, since it is possible to go from fermions to bosons and vice versa by using Jordan-Wigner transformations.
The operators P_L are defined as in equation 13.

$$P_{Li,i+1} f_i^{\sigma\dagger} f_{i+1}^{\sigma\dagger} |0\rangle = f_{i+1}^{\sigma\dagger} f_i^{\sigma\dagger} |0\rangle \tag{13}$$

After rewriting the Hamiltonian in terms of P_L and solving in the same manner as before, results now in formulas for u_12 and v_12 such that the above condition now is fulfilled.

The final expressions are shown in equations 14 and 15.

$$u_{12} = \frac{(1+e^{ik_1})(1+e^{ik_2})}{1+2e^{ik_2}+e^{i(k_1+k_2)}} \tag{14}$$

$$v_{12} = \frac{(e^{ik_1}-e^{ik_2})}{1+2e^{ik_2}+e^{i(k_1+k_2)}} \tag{15}$$

2.1.2 2D and cuprates

Cuperates are 2 dimensional, and can also be described by the t-J model. A cuprate is a material that consists of copper-oxygen layers, which possess the property that the copper d orbit is only singly occupied, whereas the oxygen p orbit is doubly occupied. The electronic structure is shown in figure 1, with to the right the simplification which is exactly the two-dimensional t-J lattice, also called the one-band model. Cuprates are of scientific interest because this group of materials is superconducting at higher temperatures then classic superconducting materials. An extensive review on the physics of cuprates starting from doping a Mott insulator is given in [7], where also the relation between cuprates and the t-J model is clearly described.

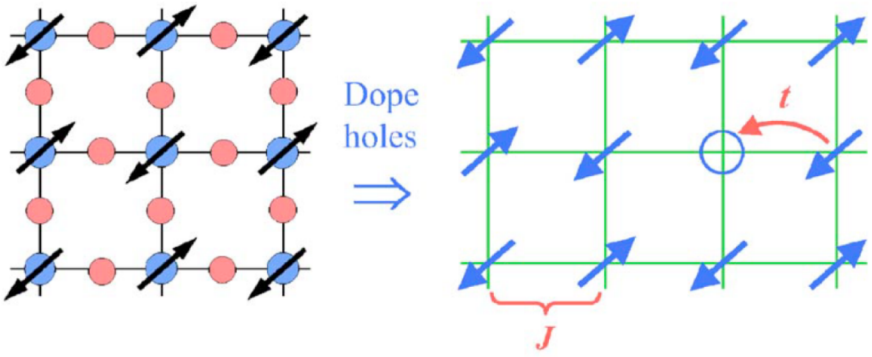

Figure 1: [7]The blue circles are copper atoms, and red is oxygen. The black arrows indicate the electron in the d orbital. The right part of the figure shows the reduction into a 2D t-J model.

The driving force behind the phase diagram in figure 2.1.2 is the strong correlation, where figure 2.1.2 shows the phase diagram of a hole-doped cuprate on the left, the right hand side shows the same, but now for electron-doping. Given the importance of the strong correlation, the t-J model is a natural fit to attempt to describe the dynamics of this class of material. Since the t-J model is in the basis a relatively simple model, there are multiple elaborations to be added, which turn out to be significant and capture some of the interesting

physics as already seen in the asymmetry of the phase diagram in figure 2.1.2. For example taking into account next-nearest neighbor hopping is important as well as electron-phonon coupling. ([7])

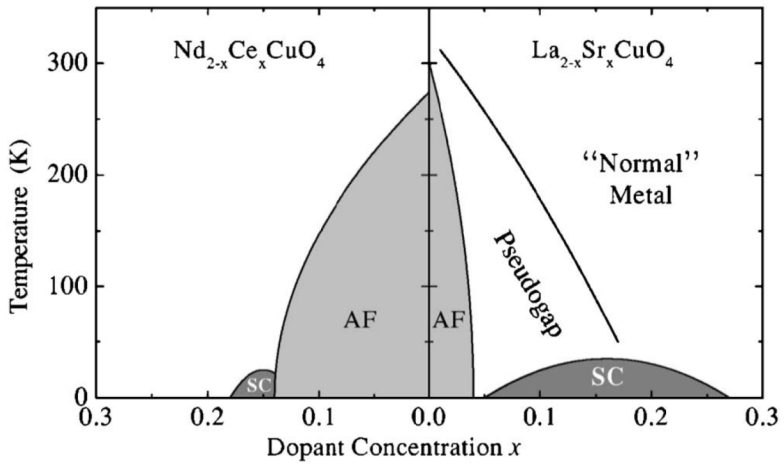

Figure 2: [7] left: Phase diagram for hole-doped cuprate; right: Phase diagram for electron-doped cuprate

2.2 Numerical methods

Over the years many methods have been used in an attempt to numerically calculate the ground state and phase transitions of the t-J model, in 1, 2 and 3 dimensions. Methods used to simulate the system are exact diagonalization [8], Densitiy Matrix Renormalization Group techniques (DMRG), Quantum Monte Carlo simulations [2] and recently also artificial neural networks have been used [3]. Of course the methods described here are not an exhaustive list, there are many more methods and variations on these methods that have been used.
The problems all methods run into when simulating the t-J model is the well known fermion sign problem. The fermion sign problem is not unique for the t-J model, it occurs whenever one attempts to do numerical calculations on a system with fermions. In short, the fermion sign problem means that when simulating fermions you have to deal with anti-symmetric wave-functions, which which results in a minus sign. This causes the errors on the simulations to increase exponentially with the system-size, the number of fermions (N). It should be noted that this problem does not occur when dealing with bosons, where the error scales with $\frac{1}{\sqrt{N}}$. Obviously, this leads to significant issues when trying to described a system with the t-J model.

2.2.1 Exact diagonalization

A frequently used method to numerically analyze the t-J model is Exact Diagonalization. ([9], [7], [8]) This method uses the Lanczos algorithm and it results in exact solutions. The exact method compared to Quantum Monte Carlo simulations or Machine learning techniques is a relatively simple, and therefore computationally less expensive.
The Lanczos algorithm is implemented in the following steps: ([8]): 1) Begin with a trial wavefunction $|\Psi_0\rangle$, 2) Apply the Hamiltonian $|\Psi_0\rangle = \epsilon_0\Psi_0 + \beta\Psi_1$, 3) To minimize the expectation value of the energy, choose the optimal linear combination of Ψ_0 and Ψ_1 by diagonalizing the matrix:

$$\begin{bmatrix} \epsilon_0 & \beta \\ \beta & \epsilon_1 \end{bmatrix}$$

4) Iterate until convergence is reached.

This method is for example used in [2], [9], [11] to calculate ground state properties.

2.2.2 Quantum Monte Carlo (QMC)

For Monte Carlo simulating the t-J model many different techniques have been used, Variational Monte Carlo ([10], [2]), exact diagonalization, Green's function Monte Carlo, and many more.
All these approaches follow a similar strategy, where first an appropriate wavefunction is found to describe the states of the system, and then simulate the system, here a lattice, using these wave-functions. So compared to classic Monte Carlo, it is much more complex due to the extra step of finding the wavefunction.
The results in [2] show that the even using complex QMC techniques the ground state of the 2D lattice can not definitively be determined, there are many states competing with one another, even in the ground state of the system.

2.2.3 Neural networks

Artificial neural networks is a machine learning tool, which is relatively new and is not routinely used to describe quantum many-body systems yet. In [3] this technique was used to learn a wave function. This machine learning method is used in an attempt to overcome the exponential complexity of the many-body wave functions, so many open questions about for example exact ground states of higher dimensional systems of interacting fermions can be answered.
Neural networks are models that connect input to output via hidden neurons, in this case a varying number of hidden neurons was used. ([3]) Here the Artificial neural network calculates the value of the wave-function, given as input a spin-configuration of the system.

The results obtained by Carleo in [3] are for the Ising and Heisenberg model in one- and two-dimensions. However, these results are very accurate for both the ground state properties as for the evolution of the spin configuration of the system, which suggests that it must also be able to find the ground state properties for the t-J model accurately.

3 Conclusion

The t-J model is a relatively simple model which despite its relative simplicity does capture a lot of interesting physics. Unfortunately, it is hard to find general solutions, even in 1D systems. In 2D no general solutions have been found yet, most recent results show competing states for the ground state, given different states with the same energy, or energy that is only slightly higher than the minimal energy.
Future research will hopefully be able to get final conclusions about general ground state properties of the t-J model in all dimensions. This would lead to attempting to solve more complex models, like a t-J model with next-nearest neighbor interaction. There is much research done on trying to solve the fermion sign problem in numerical calculations. ([13], [12]) Solving this problem would result in more accurate calculations on the t-J model.
Also the t-J model might be used in other fields of research, for example biophysics, to model collective behavior.

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