A toy model for the pseudogap state of cuprates

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A toy model is developed to capture ”dance of pre-formed pairs” in the pseudogap state of high temperature cuprate superconductors. The model is a crude description of a hypothetical situation in which spin-driven spatial organization of the pre-formed pairs is analyzed. Within a mean-field theory (a slight generalization of Bragg-Williams theory) we examined the behaviour of heat capacity and an ”order parameter” which captures the short range correlations between the pre-formed pairs. Below a transition temperature these short range correlations enhance and leads to a long range order (spin-density wave). This is examined through the breakdown of statistical independence.

Model building in physics is a first step towards understanding real complex physical systems[1]. Here, we develop an Ising type model and present its mean-field solution under Bragg-Williams approximation. This toy model gets inspiration from the pre-formed pair picture of the pseudogap state of high temperature superconducting cuprates[2]. In under-doped cuprates, as one lowers temperature (below some characteristic temperature \(T^*\)) without long range superconducting order is quite an elusive state[3]. There are many views on its origin[4, 5]. In one prominent view this electronic state is pictured as a system of pre-formed pairs but without long-range superconducting order. As one lowers the temperature below \(T_c\) these pre-formed pairs condense to give d-wave superconducting order(see for details[6]).

Here we develop a very crude model of the pseudogap state in which we assume that pre-formed pairs do exist and they interact with each other (figure 1 shows one realization from an ensemble). We will see from a mean-field type solution that below a temperature \(T_0\) (a function of the parameters of the model) some sort of long range order is established. This is analyzed in detail in the following paragraphs. The phase transition in this model is the result of a competition between thermal agitation and pair alignment due to anti-ferromagnetic exchange interaction. Virtual hoping favors an arrangement in which all the pairs align in one direction. In this case adjacent spins in each pair (depicted by an arrow in figure 1) are anti-parallel to each other and forms a low energy configuration due to exchange coupling medi-
We need to express cross terms (2nd and 4th lines in equation (1)) in terms of non-cross terms like in the 1st and 3rd lines of equation (1). From the above array (equation (2)) it is clear that we need to know 12 variables ($N^x_{RL}, N^y_{RU}, N^x_{RD}, N^y_{RU}, N^y_{UD}, etc$) and we only have eight equations. System is under-determined. For the solution, we put a reasonable approximation. Clearly the following configurations

\[ N^x_{RL} \text{ and } N^y_{UD} \]  

\[ \text{costs lots of energy (being disfavored by anti-ferromagnetic exchange).} \]

We project out these configurations from our ensemble of realizations. For this, we restrict that $k_B T << \epsilon_4$ (where $k_B$ is the Boltzmann’s constant and $T$ is the temperature). Thus, in statistical realizations in an ensemble these configurations will rarely appear, and we can assume $N^x_{RL}$ and $N^y_{UD} \approx 0$. This projection reduces the unknown variables to 10, while the system remains under-determined it is possible to write the second term in equation (1) in terms of non-cross variables. With simple algebra from equations (2):

\[ N^x_{UD} + N^y_{RL} = N^x_{RR} + N^x_{LL} + N^y_{UU} + N^y_{DD} \]

\[ - N^x_{UU} - N^x_{DD} - N^x_{RR} - N^y_{LL}. \]  

With this, the Hamiltonian takes the form:

\[ H(\epsilon_1, \epsilon_2, \epsilon_3; N^x_{RR}, \ldots) = \]

\[ - (\epsilon_1 + \epsilon_2)(N^x_{RR} + N^x_{LL} + N^y_{UU} + N^y_{DD}) \]

\[ + (\epsilon_2 + \epsilon_3)(N^y_{RR} + N^y_{LL} + N^x_{UU} + N^x_{DD}). \]  

The partition function can be calculated by summing over all possible values that these pairs can take (with constraints). Formally
We further assume that:

\[
\frac{N_{RR}}{2N} = \frac{N_{RR}}{2N} + \frac{N_{RR}}{2N} = \left( \frac{N_{RR}}{N} \right)^2
\]

The meaning of this is that "we do not have short range order apart from that which comes from long-range order" (see for details [6, 7]). We further assume that:

\[
\frac{N_{RR}^x}{2N} = \alpha \left( \frac{N_{RR}}{N} \right)^2
\]

Here \( \alpha \) varies from 0 to 1 (ensemble contains all realizations of the mixture of \( N_{RR}^x \) and \( N_{RR}^y \)). Thus

\[
\frac{N_{RR}^x}{N_{RR}^y} = \frac{\alpha}{1 - \alpha}
\]

On similar lines we have \( \frac{N_{RR}^x}{2N} \) = \( \beta \left( \frac{N_{RR}}{N} \right)^2 \) and \( \frac{N_{RR}^y}{2N} \) = \( \gamma \left( \frac{N_{RR}}{N} \right)^2 \). By writing \( N_{RR}^x \) etc in terms of \( N_R \) etc the Hamiltonian takes the following form:

\[
H(\epsilon_a, \epsilon_b; \alpha, \ldots; N_{RR}, \ldots) = 2N(N_{RR}/N)^2(\epsilon_b - (\epsilon_a + \epsilon_b)\alpha) + 2N(N_{RR}/N)^2(\epsilon_b - (\epsilon_a + \epsilon_b)\beta) + \gamma \left( \frac{N_{RR}}{N} \right)^2 \gamma \left( \frac{N_{RR}}{N} \right)^2
\]

Where \( N_D = 1 - \frac{N_{RR} + N_{LL} + N_{UU}}{N} \) (as \( N = N_{RR} + N_{LL} + N_{UU} \) + \( N_D \)). And we define \( \epsilon_a = \epsilon_1 + \epsilon_2 \), \( \epsilon_b = \epsilon_2 + \epsilon_3 \). After this mean-field approximation the partition function can simply be written as:

\[
Z(\epsilon_a, \epsilon_b; T) = \sum_{N_{RR}=0}^{N} \sum_{N_{LL}=0}^{N-N_{RR}} \sum_{N_{UU}=0}^{N-N_{RR}-N_{LL}} \int_0^1 \int_0^1 \int_0^1 d\alpha d\beta d\gamma \int_0^1 d\delta \frac{N!}{N! N_{RR}! N_{LL}! N_{UU}! (N - N_{RR} - N_{LL} - N_{UU})!} \text{e}^{-\beta H(\epsilon_a, \epsilon_b; \alpha, \ldots; N_{RR}, \ldots)}
\]

Integrals can be performed easily and the partition function takes the form:

\[
Z(\epsilon_a, \epsilon_b; T) = \frac{1}{(\epsilon_a + \epsilon_b)N} \sum_{N_{RR}=0}^{N} \sum_{N_{LL}=0}^{N-N_{RR}} \sum_{N_{UU}=0}^{N-N_{RR}-N_{LL}} \sum_{N_{RR}=0}^{N} \frac{N!}{N! N_{RR}! N_{LL}! N_{UU}! (N - N_{RR} - N_{LL} - N_{UU})!} \text{e}^{-2N\beta \epsilon_a (N_{LL}/N)^2} - \epsilon^2 - 2N\beta \epsilon_b (N_{LL}/N)^2 - 2N\beta (N_{UU}/N)^2}
\]
Williams approximation. One has to go beyond it (for example by using the renormalization group analysis\[11\]). We will see from the fluctuation behaviour of an "order parameter" that the ordered state is a highly correlated state. This means that the statistical independence (RF = \(\sqrt{<f>^2-<f>^2>} \propto \frac{1}{N}\), where f is some "order parameter"") is violated. Above the ordering temperature \(T > T_0\), statistical correlations break, and various parts of the system behave independently which leads to the resort of statistical independence. Below the ordering temperature \(T < T_0\) we get highly fluctuating phase in which the Relative Fluctuation (RF) is greater than one (rms fluctuations greater than the mean value). This seems to be independent from the lattice size as analysed below. This is a peculiarity of this phase in this toy model and may have analogies to the anomalous behaviour of the pseudogap state of cuprates (i.e., marked deviations from Fermi liquid behaviour which points towards the breakdown of adiabatic continuity\[3\]). We again stress that this is just a speculation (as no order parameter has been discovered in the pseudogap state of cuprates).

Next, we analyze the behaviour of an "order parameter" as the temperature is lowered through the transition temperature. We take \(<N_{RR}>\) as an "order parameter". \(<N_{RR}>\) is the ensemble average of the total number of two nearby right pointing arrows (arrow pairs) and \(N_{RR} = N_{RR}(\rightarrow) + N_{RR}(\leftarrow)\). We see from Fig. 3 that in the ordered phase \(T > T_0\) the average of the fraction \(\frac{N_{RR}}{N}\) (ratio between \(<N_{RR}>\) and the total number of all possible pairs \(2N\)) is about 1/4. As the temperature is increased above \(T_0\) this ratio falls, arrow pairs break (it is 0.06 at \(T = 1000 K\); thus only 6 percent of the total number of pairs are right pointing in this regime). In Fig. 4 numerical results are plotted for three lattice sizes 10 × 10, 13 × 13, and 16 × 16. The transition is sharper with larger lattice sizes (in accord with extended singularity theorem\[8\]).

Thus in the ordered phase typical configurations has more \(<N_{RR}>\) as compared to that in the disordered phase \((T > T_0)\). From this numerical calculation we also notice that \(\langle N_{RR} - N_{LL} \rangle = \langle N_{UU} - N_{DD} \rangle = 0\) and \(\langle N_R \rangle = \langle N_L \rangle = \langle N_U \rangle = \langle N_D \rangle = N/4\) at all temperatures. This means that we have equal number of right and left pointing arrows and also equal number of arrow pairs (similarly for the up and down directions). Thus our "order parameter" \(<N_{RR}>\) \((<N_{LL} > or <N_{UU}> or <N_{DD}> can also be used) do not induce directional inhomogeneity (more pairs in one direction and lesser in the opposite direction) but it captures the development of short-range pair correlations which leads to long range order in the ordered phase \((T < T_0)\)\[12\] (as analyzed below). This is the object of our study.

As \(<N_{RR}>\) \(= <N_{RR}^+> + <N_{RR}^->\) we further analyze how \(N_{RR}(\rightarrow)\) and \(N_{RR}(\leftarrow)\) behave with temperature and system parameters. Figure (4a) shows how...
\(<N_{RR}^{\gamma}\) changes with temperature (this behavior is similar to that depicted in figure (3)). From Fig. (4b) we see that majority of the pairs are \(N_{RR}^x\) (as \(\frac{<N_{RR}^x>}{<N_{RR}>} \sim 10^3\)). This is in accord with the input Hamiltonian. If we examine equation (3) we notice that the energy of \(N_{RR}^x\) is negative and \(N_{RR}^y\) pairs is positive (thus \(\rightarrow \rightarrow\) are energetically favorable). Figures (4c) and (4d) depicts how this ratio behave with \(\epsilon_2\) (i.e., the negative energy of anti-parallel pairs). As expected, this ratio increases with \(\epsilon_2\) (the parallel arrangement along the y-direction (\(\sim\)) is energetically disfavored). The trend at low temperature \((T = 100 K < T_0)\) is linear but at high temperature \((T = 1000 K > T_0)\) there is a break in the slope (Fig. 4d)). This is quite elusive. Why should the competition between \(<N_{RR}^x>\) and \(<N_{RR}^y>\) changes its nature at \(\epsilon_2 \simeq 45 \text{ meV}\) (with \(\epsilon_1 = \epsilon_2 = 20 \text{ meV}\)?)

Next we analyze the development of long range order. The fundamental thesis of Bragg-Williams approximation is: "we do not have short range order apart from that which comes from long-range order". To investigate the development of long range order from this short ranged orientational order, as the temperature is lowered through \(T_0\), we use statistical independence as a tool. We study the quantity: \(RF = \sqrt{\frac{<N_{RR}^x>-<N_{RR}^y>^2}{<N_{RR}>}}\). This is the Relative Fluctuation (RF) and is plotted in Fig. 5 as a function of temperature for three lattice sizes as shown. We see that \(T < T_0\) phase is highly fluctuating (and roughly is lattice size independent). RF is > 1 in this phase. At \(T > T_0\) RF falls with increasing temperature (Fig. 4).

For a system with short range interactions (like usual statistical mechanical systems, for example, gas in a box), relative fluctuation in some observable, say \(f\), are proportional to \(1/\sqrt{N}\):

\[
\frac{\sqrt{<f^2> - <f>^2}}{<f>} \propto \frac{1}{\sqrt{N}}
\]

Where \(N\) is the number of statistically independent units involved in the system (for example, \(f\) could be the total energy of the gas and \(N\) could be the total number of molecules present in the gas). In Figure 6 we check that how \(\frac{\sqrt{<N_{RR}^x>-<N_{RR}^y>^2}}{<N_{RR}>}\) varies with \(<N_{RR}>\). From figure (4d)) at \(T = 1491 \text{ K}\) it is clear that Statistical Independence (SI) is obeyed in the disordered phase. The validity of SI in this regime is the result of the absence of long range order (various parts of the system behave statistically independently). As the temperature is lowered we start to see deviations from statistical independence (figures 5c) and 5b)). In the ordered state (say at \(T = 301 \text{ K} < T_0\)) we see that SI is completely violated (Fig. 5a)). This clearly is the result of long range correlations (different parts of the system are statistically correlated). Thus from this analysis it is clear that the ordered state is highly fluctuating and show long range correlations. The number of ordered pairs (short range orientational order: right-right; left-left; up-up; down-down) increase in the ordered phase which leads to the long range order. The long-range order is in the form of a spin density wave. The real space structure is something like this: two spins in each arrow (one at head and the other at tail) are roughly a lattice constant away (4A in cuprates) and spins in different arrows could be many lattice spacings away (depending upon doping level). Thus there exist a fluctuating long range spin arrangement.

Further, this model reduces to simple 2-D Ising model in the following way. Let us restrict that spins can point either up or down (no left-right orientation is allowed). Then, the Hamiltonian in equation (10) will not contain terms of \(N_R\) and \(N_L\) and there will be no distinction (energetically) between \(N_{UU}^x\) and \(N_{UU}^y\), thus \(\gamma = \delta = 1\). The only energy left will be the ferromagnetic alignment energy \(-\epsilon_1\), and also the sum in equation (11) will be only over \(N_U\). The solution, un-
The solution for the model presented here leaves out many issues. One can do a better job with Bethe-Peierls approximation, or still better with Onsager’s like approach. Also the present solution does not apply at the critical point (as usual with mean-field solutions). A better job can be done using renormalization group study for this model.

In conclusion: an Ising type toy model is developed in which a “spin” can point in four possible directions in a plane. This toy model may have some analogies to the pre-formed pair picture of the pseudogap state of cuprate high temperature superconductors (however, interest here is purely mathematical). We use a slight generalization of Bragg-Williams mean-field theory to examine the behaviour of heat capacity and an “order parameter” which capture the short range correlations between the “spins” (pre-formed pairs). Below a transition temperature these short range correlations enhance and leads to a long range order which is examined through the breakdown of statistical independence.

\[ C_{\text{Onsager}} = \frac{2}{\kappa} \left( \beta \coth(2\beta \kappa) \right)^2 \left( 2 \text{Elliptic} K(\kappa) - 2 \text{Elliptic} E(\kappa) - (1 - \kappa') \left( \frac{\pi}{2} + \kappa' \text{Elliptic} K(\kappa) \right) \right) \]

\[ \kappa = \frac{2 \sinh(2\beta \epsilon)}{\cosh(2\beta \epsilon)} \] and \[ \kappa' = 2 \tanh^2(2\beta \epsilon) - 1 \]. This figure is the standard result (see figure 15.6 in [6]).

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