An Effective Field Model to High Temperature Superconductors: Fitting of The Energy Gap to the Experimental Results of the $Bi_2Sr_2CaCu_2O_8$

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ABSTRACT

We use an effective field model (transverse Ising model) to describe the dependence on the temperature of the energy gap of some two-dimensional ($2-D$) superconducting systems. The order parameter of this model is put in a direct correspondence with that of the Ising model. Then, we use the exact relations for the spontaneous magnetization of the Ising model in some $2-D$ lattices as a means to fit the experimental results of $Bi_2Sr_2CaCu_2O_8$ films obtained through reflectivity measurements by Brunel et al [Phys. Rev. Lett. 66, 1346 (1991)] and the argon-annealed $Bi_2Sr_2CaCu_2O_8$ samples investigated by Stauffer et al [Phys. Rev. Lett. 68, 1069 (1992)] through Raman scattering. The zero temperature energy gap $E_g(0)$ relations were evaluated in various $2-D$ lattices and also in the $(3-D)$ simple cubic lattice, for comparison. In the square lattice case we obtained $E_g(0) = 3.52 kT_c$, coincidentally the same number as the BCS result, and in the triangular lattice case we get $E_g(0) = 3.30 kT_c$, in agreement with the experimental findings of Brunel et al.

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As has been pointed out by Anderson: the consensus is that there is absolutely no consensus on the theory of high temperature superconductivity. Anderson attributes the novel phenomenology present on cuprates materials to a second kind of metallic state, namely, the Luttinger liquid. Schrieffer has pursued the interplay between antiferromagnetism and superconductivity, extending the BCS pairing theory beyond the Fermi-liquid regime in terms of spin polarons or "bags". As pointed out by Cox and Maple, the cuprates materials possess strong electronic correlations, where by "strong correlations" we mean that the average interaction energy substantially exceeds the average kinetic energy of the partially filled 3$d$ state of the $Cu^{2+}$ ion. Therefore the discussion of what would be the proper mechanism to describe the high temperature superconductivity in cuprates becomes polarized between the BCS theory defenders as Schrieffer, and the people who trust in the Hubbard model description as Anderson. This controversy suggest us that the proposition of new effective hamiltonians, which does not enter in specific details of the mechanism, could be an alternative way to look at this problem. Inspired in the Gorter-Casimir two-fluid model of...
superconductivity$^4$, and also taking into account the Blinc-de Gennes model$^{5,6}$ for the hydrogen-bonded ferroelectrics, Gaona J. and Silva$^7$ have proposed the following effective Hamiltonian as a means to describe some basic features of the superconducting state:

$$H = -\Omega \sum X_i - \frac{1}{2} \sum J_{ij} Z_i Z_j. \quad (1)$$

The second term of (1) is a Ising-like term, where the operator $Z$ is related to the wave function of the condensate of holes (electrons) and the coupling $J_{ij}$ favors the pairing of holes at two different lattice sites, contributing to the coherence of their wave functions below the critical temperature $T_c$. In the first term of (1) the operator $X$ is related to the wave function of the normal electrons (holes), where $\Omega$ represents the transverse field. This term, which gives dynamics to the model, could represent a mimic for the motion of the free electrons (holes) through the Fermi barrier, in close analogy with the tunneling of protons through the double-well potential barrier in the KH$_2$PO$_4$-like (hydrogen-bonded ferroelectrics) case (see$^5$).

We treat the dynamics of Hamiltonian (1), by applying the Random Phase Approximation (RPA), where we replace a time dependent expectation value < $S_i$ > by a constant part < $S_i$ > - which is just the MFA expectation value - plus a small time dependent deviation $\delta$ < $S_i$ > $e^{i\omega t}$ from the molecular field solution, to the Heisenberg equation of motion. The solution of it in the first order approximation is$^7$:

$$\omega^2 = J_0^2 < Z >^2 + \Omega \left( \Omega - J_0 < X > \right). \quad (2)$$

This solution is constrained by the zero order approximation

$$\left( \Omega - J_0 < X > \right) < Z > = 0. \quad (3)$$

Below $T_c$, $< Z > \neq 0$ and by putting (3) into(2), leads to

$$\omega_\pm = \pm J_0 < Z >. \quad (4)$$

In (4) $\omega_\pm$ can represent a two level system, and we could treat it as a gas of elementary excitations related to the hole (electron) condensate. It seems natural to interpret the separation in energy of this effective two-level system as the energy gap $E_g (T)$. We have (in units where $\hbar = 1$)

$$2\Delta (T) = E_g (T) = \omega_- (T) - \omega_+ (T) = 2J_0 < Z >. \quad (5)$$

Now, by using an idea introduced by Rummer and Ryvkin$^8$, since the quasi-particles are non-interacting fermions and their numbers are not fixed, then the averaged occupancy of the levels $\omega_\pm (T)$ is determined by the Fermi-Dirac distribution formula with zero chemical potential. Then we have

$$< n (\omega) > = \left[ e^{\beta \omega} + 1 \right]^{-1}, \quad (6)$$

where $\beta = 1/kT$. By using the above distribution and associating a $| - \rangle$ eigenstate to the $\omega_+$ energy and a $| + \rangle$ eigenstate to the $\omega_-$ energy, we obtain the following relation for the superconductor order parameter $< Z >$, namely

$$< Z > = (-1) < n_+ > + (+1) < n_- >, \quad (7)$$

or alternatively we can write

$$< Z > = \tanh \left[ (\beta J_0 < Z >) / 2 \right]. \quad (8)$$
Close to $T_c$, $< Z >$ goes to zero and we have from (8):

$$2kT_c = J_0. \quad (9)$$

At $T = 0$, $< Z > = 1$ and by putting (9) into (5) we obtain the energy gap

$$E_g(0) = 2\Delta(0) = 2J_0 = 4kT_c. \quad (10)$$

It is interesting to mention that Hao $^9$ have obtained this value for the energy gap as one of the possible solutions of the BCS $^{10}$ self-consistency equation. Equation (8) can be put in a direct correspondence with the self-consistency equation for the Ising model in the mean field approximation (MFA), but with the temperature multiplied by a factor of 2 $^{11}$. Now let us consider the situation where the thermal correlations close to $T_c$ are very important, so that the MFA is a bad description to the order parameter behavior of the system. Indeed this seems to be the case in some two-dimensional superconducting systems, as for instance the $Bi_2Sr_2CuCu_2O_8$, where the order parameter were experimentally determined through Raman scattering and reflectivity measurements $^{12, 13}$. The temperature dependence of the order parameter of the Ising model in two-dimensions is exactly known $^{14}$. We can assume that, for a two-dimensional $(2 - D)$ superconducting system where thermal correlations can not be neglected, the order parameter can be mapped into the exact relation for the spontaneous magnetization of the $2 - D$ Ising ferromagnetic model. However in this case and in the neighborhood of $T_c$, the gas of elementary excitations approximation does not work quite well and we must turn to the Boltzmann statistics. Now let us consider the exact relation for the spontaneous magnetization of the Ising model in the square lattice $^{14-16}$:

$$m = \left[ \frac{2 \tanh^2 (2\beta J) - 1}{\tanh^4 (2\beta J)} \right]^{1/8}. \quad (11)$$

In figures 1, 2 and 3, we compare eq. (11) with the experimentally determined order parameter in $Bi_2Sr_2CuCu_2O_8$ single crystals, investigated through Raman scattering by Stauffer et al. $^{12}$ and in films of the same material obtained through reflectivity measurements by Brunel et al. $^{13}$. For comparison, we plot in the same figure the eq. (8) and the BCS curve $^{10}$. We observe that the curve given by eq. (11) nicely fits to the measurements of the energy gap performed at the $Bi_2Sr_2CuCu_2O_8$ films, a manifestly $2 - D$ system. On the other hand, in the case of single crystals, the adjust to curve (11) is good in the case of the essentially $2 - D$ argon-annealed samples. In the oxygen annealed crystals the energy gap can be described both by BCS theory as equivalently by eq. (8). In fitting the experimental points to eq. (11), we have considered that:

$$m = \frac{E_g(T)}{E_g(0)} = \frac{2\Delta(T)}{2\Delta(0)}, \quad (12)$$

and in the case of eq. (8) $m$ coincides with $< Z >$.

Now let us consider the exact result for the critical temperature of the Ising model in the square lattice $^{14, 15}$. We have

$$\frac{kT_c}{J} = 2.27 \quad (13)$$

which leads to the zero temperature energy gap

$$2\Delta(T) = 2J_0 = 2zJ = \frac{8kT_c}{2.27} = 3.52kT_c. \quad (14)$$
where we took $z = 4$ (the coordination number of the square lattice). The result we got in (14), is coincidentally the same as the BCS result and must be compared with the experimental finding of $3.3kT_c$ obtained by Brunel et al.\textsuperscript{13}. It must be emphasized that although the zero temperature energy gap has been derived from a mean field analysis (eq. (5)), its use in conjunction with the exact result for $T_c$ (eq.(13)) does not lead to contradictions, once at $T = 0$, we are far from the critical temperature $T_c$, where thermal correlations are important and the mean field treatment substantially differs from the exact one.

Until now, we have compared the experimental measurements of the order parameter of the $Bi_2Sr_2CaCu_2O_8$ with the exact result of the spontaneous magnetization of the Ising ferromagnetic in the square lattice. It would be interesting to pursue further on this subject, by comparing within the same token, the zero temperature energy gap obtained by considering other $2 - D$ and $3 - D$ lattices. Therefore in the following we present the relations for the spontaneous magnetization (SM) of the Ising model in some other $2 - D$ lattices.

In the case of the honeycomb lattice\textsuperscript{17,18} we have:

$$m = \left[ \frac{1 - 2\sqrt{1 - \tanh^2(2\beta J)}}{\tanh^2(2\beta J) - 2\tanh^2(2\beta J) - 2 - 2\tanh^2(2\beta J) - 2\sqrt{1 - \tanh^2(2\beta J)}} \right]^{1/8}.$$

(15)

For the triangular lattice case, the order parameter behavior is given by the equation\textsuperscript{15,19}:

$$m = \left[ \frac{2\tanh(2\beta J) - 1}{2\tanh^3(2\beta J) - \tanh^4(2\beta J)} \right]^{1/8}.$$

(16)

In the case of the simple cubic lattice we do not have an exact relation for the SM. However, fifteen years ago, one of the present authors\textsuperscript{20} was able to "guess" a relation for the SM of this $3 - D$ lattice, which reproduces very closely the series results of Fisher\textsuperscript{21}. This relation is

$$m = \left[ \frac{3\tanh^2(3\beta J) - 1}{2\tanh^3(3\beta J)} \right]^{5/16}.$$

(17)

In table 1 we present the energy gaps of various $2 - D$ lattices. For sake of comparison the $3 - D$ simple cubic lattice is also quoted in this table.

Also is worth to notice that for the $2 - D$ lattices, the order parameter goes to zero at $T_c$ as $(T_c - T)^{1/8}$\textsuperscript{14–15,17–19}, while it behaves as $(T_c - T)^{5/16}$ in the $3 - D$ lattice\textsuperscript{20} and as $(T_c - T)^{1/2}$ in the BCS theory\textsuperscript{10} (a mean field like behavior). In figure 4 we compare the experimental data of Brunel et al\textsuperscript{13} with the exact result for the order parameter of the Ising model on the triangular lattice\textsuperscript{19}. We again obtain a nice fitting of the experimental data to the theoretical curve, with the bonus that the zero temperature gap of the theory reproduces that experimentally observed. We would like also to comment that the superconducting state of pairs of spinless quasiparticles was considered on the basis of a model hamiltonian in MFA, by Safanov\textsuperscript{22}. One of the results obtained by him is that the order parameter has a steeper rise with $(1 - T/T_c)$ in the case of parastatistics than in the case of Fermi statistics.

Finally, ultrafast dynamical optical response of $YBa_2Cu_3O_{7-\delta}$ was recently investigated by Stevens et al\textsuperscript{23}. They found that the optical response is strongly peaked at $1.5eV$, and contains two distinct components: one with a characteristic relaxation time of $\sim 5ps$, and a long-lived component ($> 10ns$) which is consistent with localized quasiparticle states at Fermi energy. For the slow component its differential transmittance behaves with the temperature as $\Delta\tau/\tau \propto \exp(-2\Delta_0/kT)$, where $2\Delta_0 = 3.5kT_c$. This corresponds to a thermal activated behavior with a fixed gap $2\Delta_0$.\textsuperscript{24}
We can interpret this experimental result of Stevens et al.\(^{23}\), taking into account that in two-dimensional systems the gap only appreciably deviates from its zero temperature value very close to \(T_c\) (see figure 1), and as we have determined in the square lattice case, this value is given by

\[2\Delta_0 = 3.52kT_c.\]

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Table 1: Zero temperature energy gap evaluated in this work for various $2 - D$ lattices and for the simple cubic lattice ($3 - D$).

| Lattice          | Transitions Temperature (values of $kT_c$ in $J$) | Zero Temperature Energy Gap |
|------------------|--------------------------------------------------|----------------------------|
| Honeycomb ($z = 3$) | 2.104 $^{[17]}$                                | 2.85$kT_c$                 |
| Square ($z = 4$)  | 2.27 $^{[14]}$                                  | 3.52$kT_c$                 |
| Triangular ($z = 6$) | 3.64 $^{[19]}$                                  | 3.30$kT_c$                 |
| Simple Cubic ($z = 6$) | 4.51 $^{[21]}$                                  | 2.66$kT_c$                 |
Figure 1, "An Effective Field Model to High Temperature Superconductors: Fitting of the Energy Gap to the Experimental Results of the Bi$_2$Sr$_2$CaCu$_2$O$_8$", E.C Bastone and P.R. Silva.
Figure 2, "An Effective Field Model to High Temperature Superconductors: Fitting of the Energy Gap to the Experimentals Results of the Bi$_2$Sr$_2$CaCu$_2$O$_8$", E.C Bastone and P.R. Silva.
Figure 3, "An Effective Field Model to High Temperature Superconductors: Fitting of the Energy Gap to the Experimental Results of the Bi$_2$Sr$_2$CaCu$_2$O$_8$", E.C. Bastone and P.R. Silva.
Figure 4, "An Effective Field Model to High Temperature Superconductors: Fitting of the Energy Gap to the Experimental Results of the Bi$_2$Sr$_2$CaCu$_2$O$_8^+$", E.C. Bastone and P.R. Silva.
Figure Captions

Figure 1: Order parameter as a function of reduced temperature $T/T_c$. The full line is the exact Ising curve for the square lattice. The points are experimental results for superconducting films of $Bi_2Sr_2CaCu_2O_8$ obtained by Brunel et al $^{13}$: open circles are obtained at $T_c = 87K$ and open squares at $T_c = 78K$. The dotted line represents the BCS theory and the crosses are the MFA results (equation (8)).

Figure 2: Order parameter as a function of reduced temperature $T/T_c$. The full line is the exact Ising curve for the square lattice. The points are experimental results for superconducting samples of $Bi_2Sr_2CaCu_2O_8$ obtained by Staufer et al $^{12}$: open circles are as-grown annealed at $T_c = 86K$, open squares are annealed in flowing Ar at $T_c = 86K$ and the triangles are annealed in $O_2$ at $T_c = 79K$. The samples are observed at $xy$ polarization. The dotted line represents the BCS theory and the crosses are the MFA results (equation (8)).

Figure 3: Order parameter as a function of reduced temperature $T/T_c$. The full line is the exact Ising curve for the square lattice. The points are experimental results for superconducting samples of $Bi_2Sr_2CaCu_2O_8$ obtained by Staufer et al $^{12}$: open circles are as-grown annealed at $T_c = 86K$, solid circles are annealed in flowing Ar at $T_c = 86K$, the triangles are annealed in $O_2$ at $T_c = 79K$. The samples are observed at $xy$ polarization. The squares are annealed in $O_2$ at $T_c = 79K$ but observed at $xx$ polarization. The dotted line represents the BCS theory and the crosses are the MFA results (equation (8)).

Figure 4: Order parameter as a function of reduced temperature $T/T_c$. The full line is the exact Ising curve for the triangular lattice. The points are experimental results for superconducting films of $Bi_2Sr_2CaCu_2O_8$ obtained by Brunel et al $^{13}$: open circles are obtained at $T_c = 87K$ and open squares at $T_c = 78K$. The dotted line represents the BCS theory and the crosses are the MFA results (equation (8)).