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INTERPRETATION FOR "HIGH"–T_c OF THE TOTALLY INTERCONNECTED SOLUTION OF THE MA AND LEE MODEL*

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ABSTRACT

The already presented totally interconnected (mean–field) approximation of the Ma and Lee model, pictures very well many ingredients of the present status of comprehension of high–T_c superconductors. The picture is that of a disordered grain with variable number of particles available for an attractive on–site pairing interaction, embedded in a reservoir of normal particles which fix the chemical potential. Interesting effect of absence of T_c and then a sharp increase and slow decay of T_c with disorder appears for weak coupling pairing as compared with the hopping probability for single particles. Interpretation is given in terms of one–particle Anderson localization theory and standard mechanisms.

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1. INTRODUCTION

In a series of papers [1]–[3] we discuss and give explicit phase diagrams within rather simple but non trivial approximations of the problematics of superconductivity and static, time–reversal symmetry obeying diagonal disorder. This line of work started from the model proposed and discussed by Ma and Lee [4]. Somewhat the question is if static, one–particle disordered hamiltonian can interpret experiments or whether the Coloumb repulsive local interaction (a many–body effect) is necessary to be taken into account. Our simple, explicit solutions seem not to contradict experiments as far as superconductivity is concerned allowing a simple discussion in terms of level scheme on a site. More sophisticated theoretical treatment (using Lie algebra techniques) on the same line, was performed by Oppermann [5] and as far as we can understand, fits rather well with what we are going to present here.

In particular we will focus on Ref. 2 where we propose and solve a model hamiltonian, in the following approximation of the Ma and Lee model. Namely, their nearest neighbour hopping term is taken by us in such a way, that any site is interconnected with every other site with equal strength. The inspiration for doing this comes from the spin glass theory and it can be thought as a mean–field treatment of Ref. 4. The other ingredients are static, diagonal, time–reversal symmetric disorder and local pairing (this is done in a standard way and was used by Bogolubov to interpret dirty alloys). Due to the recent interest in the understanding of the high–T_c compounds we think it is worth to re–interpret our model within that new problematics.

As Morgenstern [6] points out, the ingredient of *disorder* had been neglected in all theories until recent experiments of Müller et al. [7]. Also, the aspect of granular islands seems to be recognized as important. The current model used to interpret high–T_c is the extended Hubbard model. If disorder is put there on a diagonal term it falls in the line of thought appeared to that of Ref. 4. Actually, the controversy can be looked as far as the basic problem of localization theory, namely the Anderson versus Mott localization.

Introduction of disorder into a many–body problem is not currently well understood, except perhaps through specialized diagrammatic techniques. Numerical simulation gets harder when disorder is combined with the many–body problem.

Disorder was introduced in a macroscopic way, first by Ebner and Stroud [8] and then by Morgenstern [6] through models with grains in non–superconducting sea. Their approach is through the disordered arrays of Josyhsen functions described by the x–y *hamiltonian with a frustration ingredient given by the magnetic vector potential*. They characterize different phases mainly through magnetic properties and perform numerical simulation studies already developed and used for the current theories of spin glasses. The model is therefore that of disorder in a magnetic field where it seems to appear in the experiments [7].

They seem to use the same scheme for coupling phase–coherent grains with random positions and for only one grain with phase incoherence inside itself. Our interpretation for "high"–T_c of the model of Ref. 2 is done in zero field.

We also postulate a picture of a "grain" embedded in a normal reservoir of particles. Disorder is introduced in the spirit of one–particle Anderson localization theory. Namely, the "grain" is a multicomponent alloy (diagonal disorder of site energies). The interconnection (hopping) is that of a gigantic molecule with every site overlapping with every other site in the "grain" with the same strength. This is a mean–field nearest–neighbour model for the Anderson localization problem (without interactions). We fix a chemical potential (Fermi level) with a bath of non–pairing particles (which in principle also can have some pairing which is not put in the hamiltonian). Therefore, the number of carriers in the "grain", where pairing is active, is not fixed. We study explicitly the possibility of pairing of particles on the same site. The pairing interaction is only active in a certain region of energies around the fixed fermi level. As a result of the hopping term, taken in the totally interconnected approximation, the band of carriers (for which pairing can be active) shifts with respect to the fermi level in such a way that the pairing interaction cannot act upon them.

Two different behaviours are found according to whether hopping term t (normalized by the number of sites present in the grain) is stronger or weaker than the pairing interaction g. Below a critical value of t'/g (t'/g critical = .5) strong coupling pairing), the material tends to form pairs for the type of alloying (described by a square random distrobution of levels of width W) and the pairing decreases with alloying as in the standard case (as observed experimentally in general).

However, above the critical value (weak coupling) we can observe an interesting effect of no–pairing at all, until adequate W is reached, where an increase with disorder is observed due to the population of the energy region where pairing is active and then a decrease due to dilution effect.

If, on the other hand, the overlap is fixed, there will be a critical "grain" size where the effect of increase will appear; smaller grains require larger W for pairing and the increase is less pronounced (i.e. fixing t and the grain size requires rather small g).

The interpretation of this effect can be given as follows. The normal states in a "grain" are localized (either totally or at band edges). Upon alloying (W) the pairing mechanism can make itself effective due to the shift of the band *edge* towards the fermi level (a standard result in on–particle Anderson localization theory), giving a superconducting phase. Other studies [3] with a different mean–field scheme [9] give the result that in the strong–coupling regime (t'/g critical = .25) the superconducting phase is insulating. In the weak–coupling regime, on the other hand, the superconducting phase is metallic. (Within this decoupling scheme, however, we do not observe the effect described in this

paper, namely the increase of T_c with disorder, because the work was performed at a fixed number of particles).

The optimum increase is observed at the critical value and here the transition changes fron superconductor metal to metal to insulator.

2. THE MODEL

The standard Anderson model for disorder reads as follows

$$H_N = \sum_{i,\sigma}^{N} \varepsilon_i c_{i\sigma}^{+} c_{i\sigma} - t \sum_{\substack{i,i+\delta \\ \delta = x,y,z}} (c_{i\sigma}^{+} c_{i+\delta,\sigma} + c.c) \tag{1}$$

where ε_i are taken from any random distribution. Following the most standard model we use a square box distribution defined as:

$$P(\varepsilon) = \begin{cases} 1/W & \text{if } -\frac{W}{2} < \varepsilon_i < \frac{W}{2} \\ 0 & \text{otherwise} \end{cases} \tag{2}$$

This can be thought equivalent to a multicomponent alloy problem, and in particular a binary distribution could be used.

This hamiltonian has generated the whole field of study called Anderson one–particle localization. It is established now that for any W in 1-d and 2-d all states are localized and that in 3-d we get a mobility edge (transition from extended to localized states) at certain W_c and ε_c.

Due to the difficulty of the model [1] we introduced the model in the following approximation, which could be called the "interconnected model":

$$H_N = \sum_{i,\sigma}^{N} (\varepsilon_i' - \mu) c_{i\sigma}^{+} c_{i\sigma} + t' \sum_{i,j,\sigma} c_{i\sigma}^{+} c_{j\sigma} \tag{3}$$

where: $c_{i\sigma}^{+}$ is the creation operator for a particle on site i with an additional degree of freedom (σ) $\varepsilon_i' = \varepsilon_i + t'$ is the particle excitation energy $t' = t/N$ where N is the number of interconnected sites. t is the overlap of one–particle orbitals or the probabilty of hopping to another site. This last model is the mean–field model corresponding to the standard one (Eq.1).

The approximation from Eq.1 to Eq.3 is done in the same spirit as in the spin–glass theory. However, in this particular case of diagonal disorder the model can be diagonalized by an orthonormal transformation (2) which leaves the superconducting term form invariant. The normalization of the parameter t by the *size* of the interconnected

cluster is necessary in order to keep the energy an extensive quantity. Also we introduce explicitly the chemical potential (the ordered lattice). It is fixed by this bath of particles and taken in such a way that for $t' = 0$ we have a half–filled and for our pairing.

Eq.3 will describe a normal (single particle) excitation. We now add a pairing mechanism on a site (in a spirit of the standard Bogolubov theory for dirty alloys):

$$H_S = -g\Delta \sum_i^N (c_{i\uparrow}^+ c_{i\downarrow}^+ + c_{i\downarrow} c_{i\uparrow}) + g\Delta^2 N \tag{4}$$

where

$$\Delta = \frac{1}{N} \sum_i^N < c_{i\uparrow}^+ c_{i\downarrow}^+ > = \frac{1}{N} \sum_i^N < c_{i\downarrow} c_{i\uparrow} > \tag{5}$$

is the order parameter and we take $g > 0$.

In Fig. 1 we show the standard Anderson localization picture for disorder.

In Fig. 2 we show the level scheme in the interconnexion approximation.

In Fig. 3 we show the real–space lattice. In principle the two possible situations are presented, namely grains as cluster nearly in space and the other, "grains" of interconnected far away in space sites (clustering in an impurity band). The second possibility is favoured from the point of view of the localization theory since states close in energy should appear far away in real space. This second picture is the spin–glass picture.

The chemical potential $\mu = \varepsilon_F$ is fixed by the bath at $E = 0$ value. We suppose the number of carreirs low enough for not having any noticeable change when localized states approach the ε_F.

The effect of the interconnection is to shift the band by $t' = t/N$. As far as our numerical study went, no deformation was observed, neither the state at ε_F was generated.

Returning to Eq.4 we must say that the pairing (g) is most active around ε_F in a range of order g (pairing means mixing of zero and two particle levels).

As we fix the chemical potential, the number of available particles is not fixed. We have in mind that the macro–molecule is in connection with a bath of particles which are not described by the model (and which could in principle experience another type of pairing mechanism, giving a different transition temperature). The bath states are just extended states (we are thinking of a rather broad band).

In connection with high–T_c compounds we have in mind holes (or electrons) that can hop with equal probability to any site within certain regions (disordered regions). (Fig. 3). Their total number is not constant within these regions. If those "clusters" of hole states happen to form a localized band that fall close to the fermi level they will have

a tendency to pair on a site (in a singlet). The competing parameters are t' and g (hopping rate divided by the grain size and the pairing strength).

The equal probability for hopping makes the model exactly solvable. However later on we will comment on a possibility of variable range hopping (off–diagonal disorder).

We can think of a bath of normal electrons (poles) for example, which become localized within "grains" (due to disorder). These localized states can approach the Fermi level due to alloying effect (bigger W) and can form superconducting–metallic phase. The procedure to solve our model hamiltonian is standard and straight–forward and was explained in Ref. 2.

In Fig. 4 we show the interesting effect of the T_c increased by disorder (alloying).

First at low W we do not have local pairing. Increasing W the "cluster" band get broader and enters the region where the pairing interaction can be active. Strong increase of T_c is observed. After a peak, T_c decays with disorder due to the standard fact that with such a broad band, pairing a fixed number sins in a cluster, the probability of a level being close to ε_F diminishes.

In Ref. 2 we diagonalized the model hamiltonian through an orthonormal transformation which leaves the superconducting term form–invariant. For variable range hopping (off–diagonal disorder) the distribution of energy levels of the diagonalized hamiltonian can be obtained numerically. Even better, if the hopping is distributed with the Gaussian probability, we can take, due to the well known properties of this random matrix, the semi–circular distribution [10] for the energy levels.

3. DISCUSSION

We want to point out that our study started within the scheme. If the Ma and Lee model [4] which combines one–particle localization by disorder with the on–site pairing as introduced by Bogolubov for dirty superconductors. The solution to this rather difficult model is possible when interconnection between all the sites is introduced. Diagonalization for the energy was done obtaining the level distribution numerically, for the case of equal hopping (only diagonal disorder). The chemical potential was introduced as the model takes into account only localized states. Working with a fixed number of particles does not generate any interesting effects with disorder (finite cluster isolated problem). However, at fixed chemical potential we get an interesting and non common effect of an increase of the pairing T_c with disorder. This scheme corresponds to a finite "grain" in a bath of particles (coming from the left–out extended states). The effect is only observed if the strength of the pairing interaction is weaker than some critical hopping probability (which is normalized by a size of the system).

One possible interpretation is as follows. Normal electrons develop, as is well known in localization theory, localized states at band edges. Increasing disorder, the band edge approaches the middle of the "band" where the fermi level lies if the band is half-filled. There is a local pairing interaction within a small range of energies close to the Fermi level only. As localized states approach this region of energy, the pairing interaction starts to be effective and a metallic estimated metallic from other studies [8]) superconductor appears. So the increase of disorder first strongly favours the local pairing and therefore T_c increases. Then by the usual dilution effect a decrease with disorder is observed. The local pairing interaction could come from localized (also by disorder) phonons. This would mean that local pairing will only be effective (or most) for localized electrons in the same way as the usual BCS theory is worked out both for phonons and for electrons only in k-space (extended states).

Of course this only could be confirmed by specific analysis of simultaneous localization of phonons and electrons by disorder. We have tried to develop this picture some time ago (19) in a simple, standard treatment but unfortunately it was not finished with explicit results. We think it is worth trying this line of thought with some standard and single calculation because it fits within our results as interpreted through localization theory.

Another point is the importance of "grain". For not too large disorder, some electrons will go into certain regions of space into localized states and there, they will feel an attractive interaction. From localization theory we know that states close in energy are in general far away in real space. In Fig. 3a clustering effects are drawn which will lead to accumulation of charge in certain regions of real space giving raise to charge effect. We think, within our model, that rather a different type of "grains" will occur, namely as those presented in Fig. 3b where localizd states form a "band" and are spread randomly on a lattice. In this case we think that charge effects are not important.

Some preliminary results, which will be discussed elsewhere, seem to show that the pairing obtained from the Coulomb repulsion only (treated exactly) which should appear for localized states, will give T_c one order of magnitude lower (at least in mean-field treatment) than that obtained by us (2) from an explicit attractive interaction.

Up to now, we have not included any magnetic parameters in the model. In principle, it could be done within the scheme as in our preliminary work [1]. However a true glass behaviour will not be trivial to define through an order parameter as happens in the spin glass theory.

In conclusion with Oppermann's more sophisticated treatment [5] where symmetries of disorder ensembles with superconducting order are studied, there appear symmetries on the decoupled theory which explain diffusive modes. At ε_F a non-trivial symmetry results for gapless and glasslike singlet superconductor. For $\varepsilon \neq \varepsilon_F$ the symmetry changes.

Mobility edges exist inside the band of one-electron states.

As far as our understanding of this paper can go, it seems that their solution of the model (à la spin-glass) is in reasonable coincidence with our simpler approach to the totally interconnected hopping model. Of course, the same as in the spin glass theory it can be argued that the effect we observe of increase of T_c with disorder is due to the interconnection approximation and not a real effect. However the model gives a reasonable picture when looked at from the one-particle localization theory.

We think that an explicit treatment of disorder both for phonons and for electrons is needed. Preliminary numerical studies (12) with the nearest neighbour hopping term, diagonal disorder and the many-body interaction treated exactly seem to indicate the tendency for higher T_c for the attractive interaction than for the repulsive one. From Ref. 3 we get that in the weak-coupling regime superconductibity is metellic and the transition with disorder is superconducting metal – normal metal – normal insulator. From localization theory, the effect of internal mobility edge with disorder will have 3 as lower critical dimensionality.

Our study is valid for low number of "cluster" states as the chemical potential is fixed by the bath. Otherwise a self-consistent treatment is necessary. Our picture can be extended by putting several of such "grains" in a normal bath. Then the distribution of T_c (different for each "grain") could be observed. This will explain the fact that the experimental transitions are broad.

Within localization theory in 2-d all states would be localized. The effect will be observed as well is we can go as far with a mean-field treatment. In dimensionality 3 extended states would appear inside the interconnected cluster for adequate disorder. This could give raise to a transition of another temperature due to a possible coupling of localized states to extended phonon states or vice-versa. We think that the BCS type of pairing suffered by the bath itself will also appear but will not change much with not too strong disorder.

We must say that we do not aim to give this picture a true explanation of the "high-T_c" compounds. We only suggest a possible picture to get some T_c different from the usual BCS k-space pairs originated by the existence of disorder. However as this last ingredient is undoubtedly present in the "high-T_c) compounds we think our interpretation has some relevance.

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REFERENCES

[1] C. Wiecko and R. Allub, Phys. Rev. **B35**, 2041 (1986).

[2] R. Allub, A. Caro and C. Wiecko, Phys. Rev. **B36**, 8823 (1987).

[3] R. Allub, C. Wiecko and A. Caro, ICTP, Trieste, preprint IC/88/21 (1988); R. Allub, A. Caro and C. Wiecko, submitted to J.Low.Temp.Phys.

[4] M. Ma and P.A. Lee, Phys. Rev. **B32**, 5658 (1985).

[5] R. Oppermann, Europhysics Letters **3**, 431 (1987).

[6] I. Morgenstern, Z. Physik **B70**, 299 (1988).

[7] K.A. Müller, M. Takashiga and J.G. Bedrong, Phys. Rev. Lett **58**, 1143 (1987).

[8] C. Ebner and D. Stroud, Phys. Rev. **B31**, 165 (1985).

[9] R. Allub,. Phys. Rev. **B37**, 7815 (1988).

[10] E. Fradkin, private communication.

[11] C. Wiecko, Bariloche preprint (1980).

[12] G. Chiappe and C. Wiecko, "*Preliminary results*", Bariloche (1987) (unpublished.

[13] S. Kirkpatrick and T.P. Eggarter, Phys. Rev. **B6**, 3598 (1972).

Figure Caption

Fig. 1 A standard Anderson picture for one–particle localization for a random multicomponent alloy of energy level distribution of wideth W and with equal probability.

Fig. 2 The interconnected solutions. Within our numerical analysis only a shift of the box distribution appears at $t \neq 0$. As it is a mean–field approximation (∞ dimension) a mobility edge will exist. Besides, we accept the possibility of an additional state at $E = 0$. Some calculations in the past indicate this possibility (13).

Fig. 3 The regular lattice with a macro–molecular alloy described by the interconnections. For simpliocity of drawing we use 2–d. However the effect discussed requires higher dimension. a) clustering–alloy effect b) localization in an impurity band

Fig. 4 Phase diagram from Ref. 2.

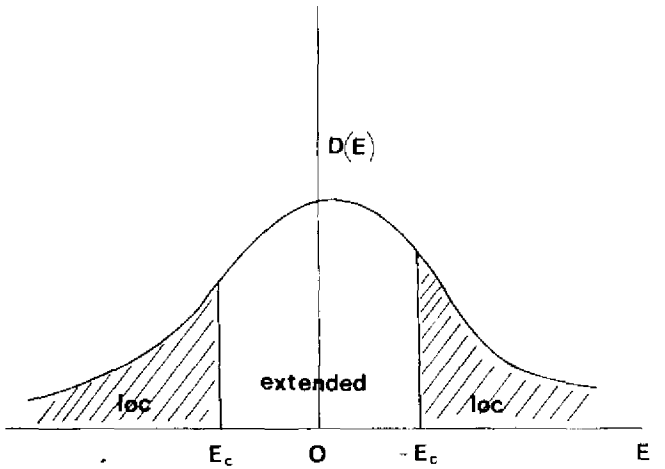
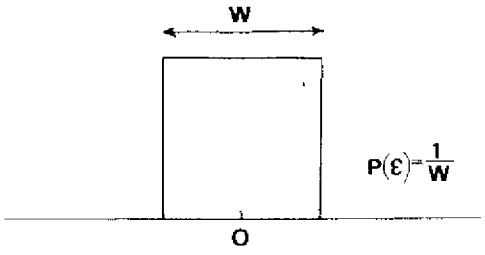
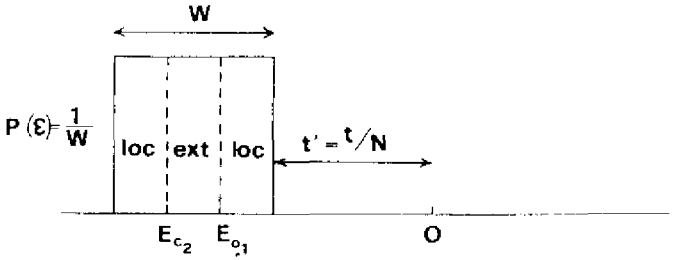


Fig.1

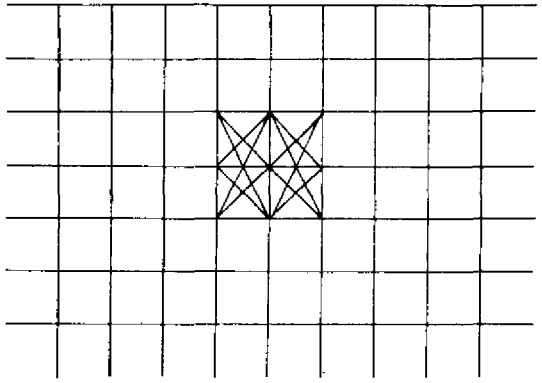


t = O

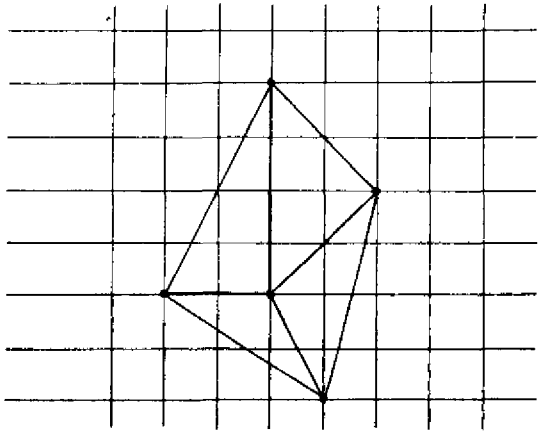


t ≠ O

Fig.2



a)



b)

Fig. 3

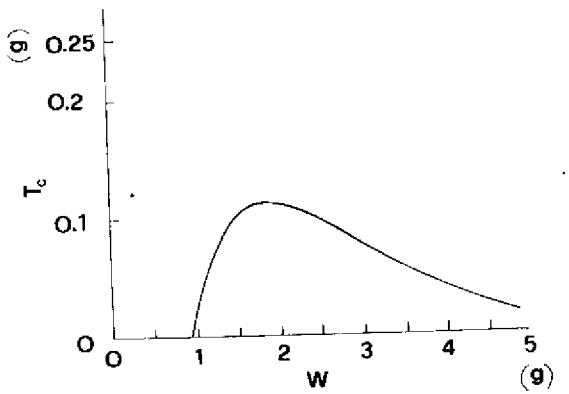


Fig.4

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