Superconductivity and random disorder in the infinite-range hopping model

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The diagonal disordered tight-binding model with infinite-range hopping and the Bardeen-Cooper-Schrieffer interaction term is solved. The results show that the zero-bandwidth limit is the mean-field approximation of the tight-binding nearest-neighbor model and that for a finite system disorder many induce superconductivity. Comparison with experimental results on amorphous alloys is made.

INTRODUCTION

Most theoretical arguments concerning superconductivity on disordered systems rely on the Anderson statement[1] that superconductivity should be insensitive to perturbations that do not destroy the time-reversal invariance. However, static disorder is known to have strong influence on the electronic states in the normal phase, such as the metal-insulator transition.[2] Consequently, superconductivity is expected to be sensitive to the crossing of the mobility edge.

It has been shown under some approximations[3] that superconductivity persists below the mobility edge, but recent experiments[4-9] have shown that T_c is strongly affected by disorder (as measured by electrical resistivity), giving a drastic reduction of T_c with increasing resistivity.

Although some authors assumed that disorder increases the Coulomb repulsion leading to a decrease of T_c,[10-12] it is also possible to study the effects of disorder alone.

Analytic results for disordered systems can easily be obtained neglecting the kinetic energy of electrons, i.e., zero bandwidth limit (ZBW). In a recent paper[13] we described the superconductivity in this limit. In spite of this rather drastic approximation, satisfactory qualitative interpretation of quite a number of different experiments was obtained.

In this paper we consider the infinite-range hopping model (IRH): that an electron may hop from a site to every other site with equal matrix element. This model is solved exactly. Although unphysical in the limit of macroscopic systems the IRH model has proved to be very fruitful in the field of spin glasses. Its analytic solution by Sherrington and Kirkpatrick[14] gave rise to a very large amount of work.

Compared to the ZBW[13] limit which represents the extreme insulator regime, one could think that the IRH should give the delocalized regime. As it is shown below this intuitive interpretation is not exact.

From the point of view of the physical meaning of the IRH model it can represent two different systems. One is a finite cluster of N particles where the size scale is of the order of the hopping range. It would illustrate a granular superconductor[15] with low probability of tunneling between grains. In what follows we shall consider these grains with a fixed number of particles or with a fixed chemical potential, each case representing different interactions with the normal matrix. When the chemical potential is kept constant this model presents the interesting feature of superconductivity induced by disorder. It means that for certain values of the parameter that define the model the critical temperature superconductivity rises with increasing disorder.

The other system that many be described with this model is through the thermodynamic limit $N \rightarrow \infty$, where the sample is embedded in an N-dimensional space. This limit gives as a result that its solution reduces exactly to that of the ZBW limit. Making an analogy with the results obtained in spin glasses where the solution of the infinite-range interaction model[14] is the mean-field solution of the model with first-neighbor interactions, we can say that the ZBW approximation is the mean-field solution of electrons with first-neighbor interactions in a disordered system.

Concerning the superconductivity we use the usual Bardeen-Cooper-Schrieffer (BCS) mean-field term Fourier transformed to site representation and define a superconductive state to exist when the spatially uniform order parameter is found.

THE MODEL

The model Hamiltonian for electrons on an hypercube of N dimensions in the tight-binding approximation is

$$H_n = \sum_{i,\sigma}^{N} (\varepsilon_i' - \mu) C_{i\sigma}^\dagger C_{i\sigma} - t' \sum_{i,j,\sigma}^{N} C_{i\sigma}^\dagger C_{j\sigma} \ . \qquad (1)$$

$C_{i\sigma}^\dagger$ is the usual creation operator of an electron on site i with spin σ; $\varepsilon_i' = \varepsilon_i + t'$ is the energy of site i plus the diagonal contribution to the hopping term; t' is included here in order to perform the sums in the second term of Eq. (1) without restrictions on i and j. The hopping term between two sites t must be renormalized to the system size $t' = t/N$ to get the energy as an extensive variable (in the thermodynamic limit). The site energies are considered as random variables taken from a given distribution $P(\varepsilon_i)$. μ is the chemical potential.

The superconductivity is described by the mean-field BCS Hamiltonian

$$H_s = -g\Delta \sum_{i}^{N} (C_{i\uparrow}^\dagger C_{i\downarrow}^\dagger + C_{i\downarrow} C_{i\uparrow}) + g\Delta^2 N \ , \qquad (2a)$$

where

$$\Delta=\frac{1}{N}\sum_i^N\langle C_{i\uparrow}^\dagger C_{i\downarrow}^\dagger\rangle=\frac{1}{N}\sum_i^N\langle C_{i\downarrow}C_{i\uparrow}\rangle \ . \tag{2b}$$

Δ is the order parameter and $g(>0)$ represents the superconductivity coupling energy.

In what follows we assume that $|\varepsilon_i|$ and t' are much smaller than the Debye energy; therefore the sum in Eq. (2) extends over all sites.

It is possible to show that the H_n Hamiltonian can be diagonalized in a new set of operators $d_{l\sigma}$, defined as $d_{l\sigma}=\sum_j u_{jl}C_{j\sigma}$. The u_{jl} are the elements of a real orthogonal matrix. H_n is diagonalized into a set of single-particle levels $\varepsilon_l^*(N)$ provided the u_{jl} satisfy the equations

$$(\varepsilon_l^*-\varepsilon_i'+\mu)U_{il}=-t'\sum_j^N U_{jl} \ . \tag{3}$$

The solutions of Eq. (3) are

$$(t')^{-1}=\sum_i^N(\varepsilon_i'-\mu-\varepsilon_l^*)^{-1} \ , \tag{4}$$

$$U_{il}=(\varepsilon_i'-\mu-\varepsilon_l^*)^{-1}\left[\sum_j^N(\varepsilon_j'-\mu-\varepsilon_l^*)^{-2}\right]^{-1/2} \ . \tag{5}$$

The fact that U_{jl} is a real transformation allows us to also diagonalize the superconducting Hamiltonian H_s. The total Hamiltonian H_n+H_s can be written in a site-diagonal form:

$$H=H_n+H_s \ ,$$

$$H=\sum_{l\sigma}^N\varepsilon_l^* d_{l\sigma}^\dagger d_{l\sigma}+g\Delta^2N-g\Delta\sum_l^N(d_{l\uparrow}^\dagger d_{l\downarrow}^\dagger+\text{H.c.}) \ . \tag{6}$$

It is clear that in the Hamiltonian (Eq. 6) the sites are coupled only through the mean-field parameter Δ (to be determined from the minimum of the total free energy). The Hamiltonian is now diagonalized for each site.

If we define

$$H_l=\varepsilon_l^*\sum_\sigma d_{l\sigma}^\dagger d_{l\sigma}+g\Delta^2-g\Delta(d_{l\uparrow}^\dagger d_{l\downarrow}+\text{H.c.}) \tag{7}$$

the eigenstates of the Hamiltonian are (a) two one-particle states $d_{l\sigma}^\dagger|0\rangle$ with energy $\varepsilon_l^*+g\Delta^2$ and (b) two states mixing zero and two particles (a linear combination of $|0\rangle$ and $d_{l\uparrow}^\dagger d_{l\downarrow}^\dagger|0\rangle$) with energies

$$(g\Delta^2+\varepsilon_l^*)\pm\sqrt{\varepsilon_l^{*2}+g^2\Delta^2} \ .$$

The free energy for a site l is

$$\begin{aligned}F_l&=-\beta^{-1}\ln(Z_l)\\&=-\beta^{-1}\ln\{2\exp[-\beta(g\Delta^2+\varepsilon_l^*)]\\&\qquad\times[1+\cosh(\beta\sqrt{\varepsilon_l^{*2}+g^2\Delta^2})]\} \ .\end{aligned} \tag{8}$$

Using the "quenched-type" average[16] we get

$$F=\sum_l\langle F_l\rangle=N\langle F_l\rangle=N\int P(\varepsilon_l^*)F_l(\varepsilon_l^*)d\varepsilon_l^* \ . \tag{9}$$

Considering the random variable ε_i, uniformly distributed between $-W/2$ and $W/2$, and Eq. (4), it can be shown that $P(\varepsilon_l^*)$ becomes

$$P(\varepsilon_l^*)=\begin{cases}1/W \text{ if } -\dfrac{W}{2}+t'-\mu\le\varepsilon_l^*\le\dfrac{W}{2}+t'-\mu \ ,\\ 0 \text{ otherwise} \ .\end{cases}$$

Equation (9) reads

$$F=-\frac{N}{\beta}\ln(2)+Ng\Delta^2+Nt' -\frac{N}{\beta}\frac{1}{W}\int_{-W/2+t'-\mu}^{W/2+t'-\mu}d\varepsilon^*\ln[1+\cosh(\beta\sqrt{\varepsilon^{*2}+g^2\Delta^2})] \ . \tag{10}$$

From this expression for the free energy the superconducting normal second-order transition temperature T_c is ob-

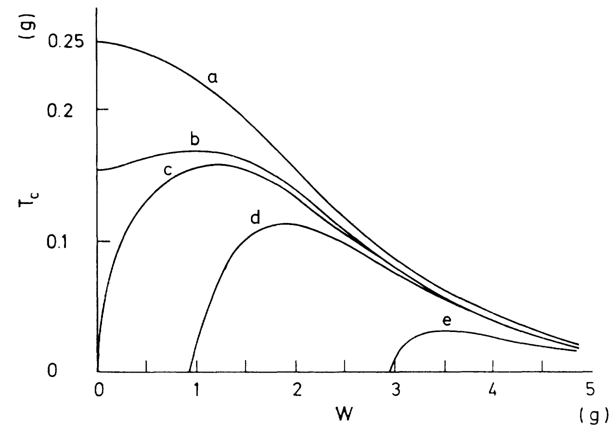

FIG. 1. Variation of the critical temperature (T_c) with disorder (W) according to Eq. (11) for the hopping term (t') ranging from 0 to 1.5. (a) $t'=0$; (b) $t'=0.45$; (c) $t'=0.5$; (d) $t'=0.7$; (e) $t'=1.5$. Measuring energies in units of the superconductivity coupling energy (g).

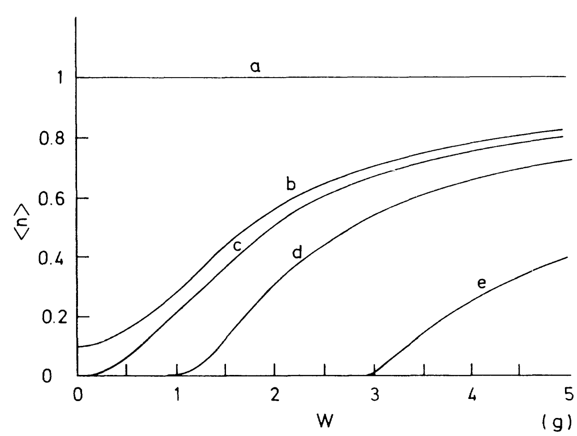

FIG. 2. Variation of the average number of particles per site $\langle n\rangle$ with disorder (W) according to Eq. (12). The hopping term (t') ranging from 0 to 1.5, corresponding to the same values as in Fig. 1.

tained solving

$$1=\frac{g}{2W}\int_{-W/2}^{W/2}\frac{d\varepsilon}{(\varepsilon+t'-\mu)}\tanh\left[\frac{\varepsilon+t'-\mu}{2T_c}\right] . \quad (11)$$

Also the average number of particles per site is obtained from

$$1-\langle n\rangle=\frac{2}{\beta W}\ln\left[\frac{\cosh\{\beta/2[(W/2)+t'-\mu]\}}{\cosh\{\beta/2[-(W/2)+t'-\mu]\}}\right] . \quad (12)$$

We proceed to analyze the case $\mu=0$.

Numerical solutions of Eq. (11) for T_c/g as a function of W/g for several values of t'/g are shown in Fig. 1. Figure 2 shows $\langle n\rangle$ as a function of W/g for the same values of t'/g.

DISCUSSION

In order to get analytic results we shall consider two limit cases, $W/g\ll 1$ and $W/g\gg 1$. In the limit of small disorder ($W/g\ll 1$) Eqs. (11) and (12) can be written as

$$1=\frac{g}{2t'}\tanh\left[\frac{t'}{2T_c}\right] , \quad (13a)$$

$$\langle n\rangle=1-2\frac{t'}{g} . \quad (13b)$$

Equation (13a) has solutions only if $0\le t'/g\le 1/2$. In the limit $t'/g\to 0$ we recover the result of the ZBW limit $T_c=g/4$ together with $\langle n\rangle=1$. Increasing the hopping leads to a decrease of the transition temperature down to zero for $t'/g=\frac{1}{2}$ and a corresponding decrease of $\langle n\rangle$ which is zero for $T_c=0$. In the case of $t'/g>\frac{1}{2}$, the system contains no electrons and $T_c=0$ in the limit of vanishing disorder.

The second case $W/g\gg 1$, strong disorder, usual approximations in the integral appearing in Eq. (11) give

$$T_c=0.5[(W/2)^2-t'^2]^{1/2}\exp[1-(W/g)] , \quad (14a)$$

while Eq. (12) gives

$$\langle n\rangle=1-2\frac{t'}{W} . \quad (14b)$$

Equation (14a) gives an exponential decay of the transition temperature with increasing disorder. The validity of this result is restricted to the condition $t'<W/2$. Observation of Fig. 1 indicates that this condition is always fulfilled in the cases of interest.

Finally it is interesting to analyze the case $t'/g>\frac{1}{2}$. From Fig. 1 we observe that a finite amount of disorder is necessary to induce superconductivity. Analytically this critical disorder W_c corresponding to a given value of the hopping t' is given by the solution of

$$t'\simeq\frac{W_c}{2}\coth\left[\frac{W_c}{g}\right] . \quad (15)$$

For $t'/g\gtrsim\frac{1}{2}$ it reduces to

$$W_c\simeq g\{6[(t'/g)-\tfrac{1}{2}]\}^{1/2} , \quad (16)$$

and in the case $t'/g\gg 1$

$$W_c\simeq 2t' , \quad (17)$$

and whenever $T_c=0$ in this regime, $\langle n\rangle$ is also zero. The conclusion of the analysis is that the effects of the disorder in a system with hopping t' can be classified in two regimes. For $t'<g/2$ the disorder starts increasing the T_c with null derivative at $W=0$ to decay exponentially at large disorder. Consequently, T_c reaches a maximum at some value of disorder. For $t'\ge g/2$ the ordered system has no electrons and the superconductivity may be induced if the disorder is large enough. Further increase of W makes T_c reach a maximum to die off exponentially at $W\gg g$.

From the definition of t' ($t'=t/N$) the thermodynamic limit implies $t'\to 0$. In this limit Eq. (11) reproduces exactly the result of the zero band-width model[13] (ZBW). This conclusion suggests a natural interpretation of the ZBW: The infinite-range interaction model is equivalent to the mean-field approximation to the tight-binding diagonal disorder nearest-neighbors model, and in the thermodynamic limit gives the same result as the ZBW model. Therefore the ZBW model is the mean-field approximation of the tight-binding diagonal disordered nearest-neighbors model

Now let us analyze the case $\mu\neq 0$ in such a way that $\langle n\rangle=1$ regardless of the values of t' and W. From Eq. (12) $\langle n\rangle=1$ implies $\mu=t'$, which, replaced in Eq. (11), gives T_c independent of the value of t' and equal to that obtained in the preceding analysis with $t'=\mu=0$, i.e., curve a in Fig. 1.

In other words if the system conserves the number of particles then the infinite-range hopping model reduces exactly to the ZBW limit not only in the thermodynamic limit but for any sample size.

From the point of view of the qualitative microscopic interpretation of the effects of t' and W, in the case of a fixed chemical potential, let us see what happens on a particular site. In this model the superconductivity is essentially the result of a quantum mixture of zero- and two-particle states. This mixture is optimized when the two states are degenerate ($\Delta=\frac{1}{2}$). Without disorder, the effect of t' is to split the zero and two-particle levels weakening the superconductivity ($\Delta<\frac{1}{2}$), leading to a complete destruction for $t'=g/2(\Delta=0)$.

For a given t' and small disorder ($W<t'$) the splitting between zero- and two-particle states is reduced in some sites and increased in others, giving a net result of an enhanced superconductivity.

For large disorder ($W>2t'$) the decreasing number of sites where the pair formation is factored leads to a net reduction of the critical temperature.

The existence of a maximum of T_c at some disorder $W\neq 0$ is an experimental fact observed, for instance, in several zirconium-based amorphous transition-metal alloys.[17] These observations are usually explained in terms of the electrons per atom ratio rules,[18] which are supposed to reflect the dependence of the electron density of states at the Fermi level in the alloy. However, these explanations are not completely satisfactory and perhaps a contribution of the effect outlined in this work is also present.

Besides the existence of the maximum, the exponential decay of T_c at large disorder is in good agreement with experimental results.[6] The theoretical model used in Ref. 6 to fit the experimental data[19] based on an enhanced Coulomb repulsion, fails to explain the decrease of the rate of the T_c depression as disorder increases. Our result suggests that the effect of disorder alone could account for the experimental observations, although the simplicity of our model prevents us from a quantitative comparison.

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