

T_c calculation of disordered superconductor with local electron pairing

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Starting with an effective hamiltonian describing a disordered substitutional alloy superconductor with local electron pairing, we derive a random version of the Gorkov equations in the weak coupling limit. The disorder is treated by means of the coherent potential approximation. We take special care of the energy dependence of the order parameter as introduced by averaging. This leads to a complex wave function renormalisation parameter Z similar to that found in strong coupling theory. The transition temperature T_c is calculated analytically for the lorentzian density of states of the host metal. The numerical calculation of T_c has been performed for a range of phenomenologically important parameters such as alloy concentration, relative position of (random) atomic levels, value of on-site effective attraction and carrier density for the densities of states suitable for $d=2$ and $d=3$ spatial dimensions and bipartite lattices.

1. Introduction

In the BCS theory of superconductivity the electrons are paired in k -space as originally proposed by Cooper [1]. The opposite limit of pairing in real space has been discussed by Schafroth and others even before BCS theory [2]. The material in which Schafroth scenario of “small” pairs is realized, is sometimes called a local pair (LP) superconductor. The reader is referred to the recent review [3] for discussion of LP superconductivity-model systems, properties and origin of strong local attraction leading to LPs. For the purpose of this work we postulate the existence of the effective hamiltonian appropriate for the description of a superconductor with local electron pairing. To this end we take the widely used negative U Hubbard model. Such a model has been extensively studied [3] both in weak $|U| \ll t$ [4] and strong [5] $|U| \gg t$ coupling limits. This model (or its generalization including additionally the intersite Coulomb repulsion) has been used by several authors as a model for superconductivity (and CDW) in doped BaBiO_3 ($\text{BaPb}_{1-x}\text{Bi}_x\text{O}_3$,

$\text{Ba}_{1-x}\text{K}_x\text{BiO}_3$) [3,6–8] and in the newly discovered superconducting fullerenes M_xC_{60} [9]. The two-dimensional version of the model has also been discussed in the context of the effective description of the superconductivity in Cu–O planes of superconducting copper oxides [10]. Doping of the materials both outside and inside Cu–O planes has an important impact on the superconductivity. Doping outside the CuO plane introduces holes into the plane and the materials start to be metallic and superconducting. It certainly also introduces disorder to the CuO planes in the sense of changing local values of parameters. The doping in the Cu–O planes introduces much more disorder.

It is the purpose of this work to study the random version of the negative U -Hubbard model describing a substitutionally disordered alloy superconductor.

The organization of the paper is as follows. In section 2 we describe the model, and derive the random version of the Gorkov–BCS equations. Section 3 deals with the averaging. We use the single-site coherent potential approximation CPA approach in its analytical version. The metal–insulator transition as

well as the dependence of T_c on various parameters of our model will be studied in section 4. In section 5 we summarize our weak coupling results, discuss the previous work in the strong coupling limit and the possible extensions of the present model.

2. The model and equations of superconductivity

We shall start with the following hamiltonian in the tight binding representation [3]

$$H = \sum_{j\sigma} t_{ij} a_{i\sigma}^+ a_{j\sigma} + \sum_{i\sigma} (\epsilon_i^0 - \mu) a_{i\sigma}^+ a_{i\sigma} - \sum_i U_i n_{i\downarrow} n_{i\uparrow}. \quad (1)$$

Here t_{ij} is the (nearest-neighbor) hopping integral, μ is the chemical potential, ϵ_i^0 , U_i are random, in general, site energy and on-site effective attraction. The periodic model is obtained by assuming $\epsilon_i \equiv 0$ and $U_i = U$. The parameter U of the effective instantaneous attraction between electrons of opposite spins does not possess any cut-off different from the bandwidth. This means that the description of the thermodynamics of the superconductor with local electron pairing requires the knowledge of the relevant function, e.g. density of states for all energies and not only in the vicinity of the Fermi energy E_F ($E_F = \mu(T=0 \text{ K})$).

There may be a number of reasons for the fluctuation of ϵ_i^0 and U_i . The most obvious is a substitutionally disordered $A_{1-x}B_x$ alloy, where the parameters ϵ_i^0 and U_i take on values ϵ_A^0 , ϵ_B^0 and U_A , U_B depend on the kind of atom occupying the site i . The corresponding probability distribution for the $A_{1-x}B_x$ alloy is assumed to be

$$p(\gamma_i) = (1-x)(\gamma_i - \gamma_A) + x\delta(\gamma_i - \gamma_B), \quad \gamma_i = \epsilon_i^0, U_i. \quad (2)$$

Model (1) as it stands may be used in $d=3$ as well as $d=2$ spatial dimensions depending on the geometry of the underlying lattice of sites (i, j) . Here we shall assume the hopping integrals to be periodic in the lattice and taking on a nonzero value $-t$ for nearest-neighbor sites. Thus the energy spectrum

$$\epsilon_k = -t \sum e^{ik\delta}, \quad (3)$$

where the sum goes over nearest-neighbors of the

central site, and the wave vector k will be $d=3$ or $d=2$ dimensional. The rest of the problem is local and thus independent of dimensionality.

The equations of superconductivity will be derived here by means of the equation of motion for the two-time thermodynamic Green's function (GF). It is a matrix $\hat{G}_{ij}(\omega)$ in the Gorkov–Nambu representation [11]

$$\hat{G}_{ij}(\omega) = \begin{bmatrix} \langle\langle a_{i\uparrow} | a_{j\uparrow}^+ \rangle\rangle_\omega & \langle\langle a_{i\uparrow} | a_{j\downarrow} \rangle\rangle_\omega \\ \langle\langle a_{i\uparrow}^+ | a_{j\uparrow} \rangle\rangle_\omega & \langle\langle a_{i\downarrow}^+ | a_{j\downarrow} \rangle\rangle_\omega \end{bmatrix}. \quad (4)$$

The equation of motion

$$\begin{aligned} \omega \langle A | B \rangle_\omega &= [A, B]_\eta + \langle\langle [A, H] / B \rangle\rangle_\omega \\ &= \langle [A, B]_\eta \rangle - \langle\langle A | [B, H] \rangle\rangle_\omega, \end{aligned} \quad (5)$$

applied to $\hat{G}_{ij}(\omega)$ and a Hartree–Fock–Bogolubov type of factorisation leads to the expression

$$\sum_\tau \begin{bmatrix} (\omega - \epsilon_i + \mu)\delta_{i\ell} - t_{i\ell} & A_i \delta_{i\ell} \\ A_i^+ \delta_{i\ell} & (\omega + \epsilon_i - \mu)\delta_{i\ell} - t_{i\ell} \end{bmatrix} \hat{G}_{ij}(\omega) = \hat{\tau}_0 \delta_{ij}. \quad (6)$$

where we have defined

$$A_i = U_i \langle a_{i\downarrow} a_{i\uparrow} \rangle, \quad A_i^+ = U_i \langle a_{i\uparrow}^+ a_{i\downarrow}^+ \rangle, \quad (7)$$

$$\epsilon_i = \epsilon_i^0 - U_i \langle n_i \rangle, \quad (8)$$

and

$$\langle n_{i\uparrow} \rangle = \langle n_{i\downarrow} \rangle \quad (9)$$

From the spectral representation one finds

$$A_i = -\frac{U_i}{\pi} \int_{-\infty}^{\infty} d\omega \frac{\text{Im} G_{ii}^{12}(\omega + i0)}{e^{\beta\omega} + 1}. \quad (10)$$

In the following we use the notation

$$\hat{G}_{ij} = \begin{bmatrix} G_{ij}^{11} & G_{ij}^{12} \\ G_{ij}^{21} & G_{ij}^{22} \end{bmatrix} \quad (11)$$

and the symmetry properties (for complex ω)

$$\begin{aligned} G_{ij}^{22}(\omega) &= -G_{ij}^{11*}(-\omega^*), \\ G_{ij}^{21}(\omega) &= G_{ij}^{12*}(-\omega^*). \end{aligned} \quad (12)$$

The chemical potential μ is not a proper thermodynamical variable in a system with no cut-off interaction parameters. It has thus to be eliminated in favour of the carrier concentration n . The corre-

sponding condition for the average number of carriers in the system to be n is defined in terms of the averaged Green function \bar{G} (see eq. (19) below) and reads

$$n = -\frac{2}{\pi} \int_{-\infty}^{\infty} d\omega \frac{\text{Im} \bar{G}^{11}(\omega + i0)}{e^{\beta\omega} + 1}, \quad n \in [0, 2]. \quad (13)$$

Equations (6)–(10) describe both normal (diagonal terms) and superconducting (off-diagonal terms) properties of the system. For disordered alloys the Green's function (11) is not transitionally invariant, the Fourier transformation is not allowed and in order to get experimentally meaningful results one has to average over possible configurations. In a coherent potential approximation [12] this is done by requiring vanishing of the average scattering matrix for a single impurity embedded in an otherwise averaged medium. The procedure is described in the next section. Let us, however, note that the absence of the (already mentioned) energy cut-off for the attractive interaction makes this approach different from the previous calculations for disordered BCS superconductors [13,14].

3. The configurational averaging

Let us introduce the averaged GF, to be denoted by \bar{G} . By definition it is periodic, and its Fourier transform may be written as

$$\bar{G}(z) = \frac{1}{N} \sum_{\mathbf{k}} (z\hat{\tau}_0 - (\epsilon_{\mathbf{k}} - \mu)\hat{\tau}_3 - \hat{\Sigma}(z))^{-1}, \quad (14)$$

where $\hat{\Sigma}(z)$ is a yet undefined (matrix) coherent potential, and $\hat{\tau}_i$ the Pauli matrices. The off-diagonal terms of Σ play the role of the order parameter for the averaged system. The appearance of a nonzero value for σ^{12} and G^{12} below some characteristic temperature T_c marks the onset of superconductivity. The CPA for the determination of the $\Sigma(z)$ is the vanishing of the averaged value of the single-site scattering operator \hat{T}_i [12]

$$\langle \hat{T}_i \rangle \equiv (1-x)\hat{T}_A + x\hat{T}_B = 0, \quad (15)$$

where $\hat{T}_i = \hat{V}_i(1 - \bar{G}\hat{V}_i)$ and the ‘‘scattering’’ potential \hat{V}_i is given by

$$\hat{V}_i = \begin{bmatrix} \epsilon_i - \Sigma_{11}(\omega), & -D_i + \Sigma_{12}(\omega) \\ -D_i^* + \Sigma_{21}(\omega), & -\epsilon_i + \Sigma_{22}(\omega) \end{bmatrix}. \quad (16)$$

Equation (15) is the condition for the determination of $\Sigma(z)$ which plays here the role of (and is sometimes so called) the self-energy in many body theories.

From the configurationally averaged Green's function (14) written in the form

$$\bar{G}(\omega) = \frac{1}{N} \times \sum_{\mathbf{k}} \begin{bmatrix} \omega - \Sigma_{11}(\omega) + \mu - \epsilon_{\mathbf{k}}, & \Sigma_{12}(\omega) \\ \Sigma_{21}(\omega), & \omega + \Sigma_{22}(\omega) - \mu + \epsilon_{\mathbf{k}} \end{bmatrix}^{-1} \quad (17)$$

and the symmetries (12) we read off the symmetry properties of the $\hat{\Sigma}$ elements

$$\begin{aligned} \Sigma_{22}(\omega) &= \Sigma_{11}^*(-\omega^*), \\ \Sigma_{21}(\omega) &= \Sigma_{12}^*(-\omega^*). \end{aligned} \quad (18)$$

CPA condition (15) can be shown to be equivalent to the condition

$$\bar{G}(\omega)(1-x)\bar{G}_A(\omega) + x\bar{G}_B(\omega), \quad (19)$$

where the conditionally averaged GF \bar{G}_i is defined by

$$\bar{G}_i(\omega) = \bar{G}(\omega) + \bar{G}(\omega)V_i(\omega)\bar{G}_i(\omega)$$

or

$$\bar{G}_i(\omega) = \bar{G}^{-1}(\omega) - V_i(\omega)^{-1}. \quad (20)$$

If we define $\hat{\Sigma}_{12}$ as

$$\hat{\Sigma}_{12}(\omega) = \frac{2\omega}{2\omega + \Sigma_{11}^*(-\omega^*) - \Sigma_{11}(\omega)} \Sigma_{12}(\omega) \quad (21)$$

then from eq. (17) can be found the very important exact relation

$$\bar{G}_{12}(\omega) = -(\bar{G}_{11}(\omega) - \bar{G}_{11}^*(-\omega^*))\hat{\Sigma}_{12}(\omega). \quad (22)$$

Using eqs. (16) and (21) we get

$$G_{11}^i(z) = \frac{1}{-D_i(z)} \left(\frac{\bar{G}^{11}(z)}{-d(z)} - \epsilon_i + \Sigma_{11}^*(-z^*) \right) \quad (23)$$

$$G_{12}^i(z) = \frac{1}{-D_i(z)} \left(\frac{\bar{G}^{12}(z)}{-d(z)} - D_i + \Sigma_{12}(z) \right), \quad (24)$$

where we have denoted $d(z) = \det \bar{G}$, $D_i(z) = \det \bar{G}_i$ with respective symmetries

$$d(z) = d^*(-z^*), \quad D_i(z) = D_i^*(-z^*). \quad (25)$$

Hence using symmetries of eqs. (12, 18, 25) and the relation (22) in the CPA conditions (15, 19) we get

$$\bar{\Sigma}_{12}(z) = \frac{\langle \Delta_i(G_{11}^i(z) - G_{11}^{i*}(-z^*)) \rangle}{\bar{G}_{11}(z) - \bar{G}_{11}^*(-z^*)}, \quad (26)$$

$$G_{12}^i(z) = -\frac{G_{11}^i(z) - G_{11}^i(-z)}{2z} \bar{\Sigma}_{12}(z) - \frac{1}{D_i(z)} (\bar{\Sigma}(z) - \Delta_i). \quad (27)$$

The spectral representation (10) leads to the following exact equation for $\bar{\Sigma}_{12}$:

$$\bar{\Sigma}_{12}(z) = -\left\langle \frac{G_{11}^i(z) - G_{11}^{i*}(-z^*) U_i}{\bar{G}_{11}(z) - \bar{G}_{11}^*(-z^*) \pi} \times \int d\omega \operatorname{th}(\beta\omega/2) \operatorname{Im} \left(\frac{G_{11}^i(\omega)}{2\omega} \bar{\Sigma}_{12}(\omega) - \frac{1}{D_i(\omega)} (\bar{\Sigma}_{12}(\omega) - \Delta_i) \right) \right\rangle. \quad (28)$$

From the CPA conditions (15) or (19) it is easy to obtain the second equation for $\bar{\Sigma}$:

$$(1-x)\hat{V}_A + x\hat{V}_B = \hat{V}_B \bar{G} \hat{V}_A \quad (29)$$

We need only an equation for Σ_{11} and it is given by the (1,1) element of matrix equation (29). The (1, 2) element is explicitly given by eq. (28). Equations (10, 13, 28) and (29) form a set (exact in the Hartree-Fock-Bogolubov and CPA schemes) of equations for the determination of normal state and superconducting properties of the system. In the following we describe additional approximations we do and the scheme of calculations for both $d=3$ and $d=2$ systems.

4. Results and discussion

4.1. Main approximations

For a given value of the chemical potential the local electron occupancies n_A , n_B are given by

$$n_{A,B} = \int_{-\infty}^{\infty} \rho_{A,B}(\epsilon) f(\epsilon) d\epsilon, \quad (30)$$

where $f(\epsilon)$ is the usual Fermi distribution function and $\rho_{A,B}$ is the local density of states at an A or B site

$$\rho_{A,B}(\epsilon) = -\frac{2}{\pi} \operatorname{Im} g_{A,B}(\epsilon + i0). \quad (31)$$

The averaged site occupation n and density of states $\rho(\epsilon)$ can be expressed as

$$n = \langle n_i \rangle = (1-x)n_A + xn_B, \quad \rho(\epsilon) = \langle \rho_i(\epsilon) \rangle = (1-x)\rho_A(\epsilon) + x\rho_B(\epsilon). \quad (32)$$

It is obvious that the parameter n calculated in an alloy has to be equal to the density of free carriers in the system. This in turn depends on the chemical nature of the constituents forming an alloy. Let denote by n_A^0 , n_B^0 the number of valence electrons per atom in the system composed of only atoms of type A or B. In an $A_{1-x}B_x$ alloy the concentration n is

$$n = (1-x)n_A^0 + xn_B^0.$$

n_A^0 , n_B^0 are material parameters like ϵ_A^0 , ϵ_B^0 . In this work we take $n_A^0 = 0$, $n_B^0 = 2$, similarly as in refs. [7] and [8].

Equation (32) for n together with eqs. (30) and (31) reduces to the condition (13) for the determination of μ . The diagonal part of the self-energy $\Sigma_{11}(z)$ can be, in the first approximation, calculated by neglecting the effect of superconductivity on it (i.e. the terms proportional to $\Sigma_{12}(z)$). Thus it is given by the solution of

$$\Sigma_{11}(z) = (1-x)\epsilon_A + x\epsilon_B - (\epsilon_A - \Sigma_{11}(z))\bar{G}_{11}(z)(\epsilon_B - \Sigma_{11}(z)). \quad (33)$$

This approximation is certainly valid for the calculation of T_c where both Σ_{12} and \bar{G}_{12} are small compared to Σ_{11} and \bar{G}_{11} . In the spirit of the weak coupling we neglect the last term on the rhs of eq. (27) for $\bar{\Sigma}_{12}$. It takes thus the form

$$\bar{\Sigma}_{12}(z) = -\left\langle \frac{G_{11}^i(z) - G_{11}^{i*}(-z^*)}{\bar{G}_{11}(z) - \bar{G}_{11}^*(-z^*)} \right\rangle$$

$$\times \frac{U_i}{\pi} \int d\omega \operatorname{th}\left(\frac{\beta\omega}{2}\right) \operatorname{Im}\left(\frac{G_{11}^i(\omega)}{2\omega} \bar{\Sigma}_{12}(\omega)\right) \Bigg\rangle. \quad (34)$$

Let us note that our treatment of disorder leads to a frequency dependent order parameter. This result has been previously derived in the context of BCS [13] and Eliashberg [14] theories of superconductivity in disordered alloys. In this work we study the superconducting transition temperature so we need only the linearized order parameter equation. This means that the Green's functions entering eq. (34) are to be calculated for $\Sigma_{12}=0$:

$$G_{11}^i(z) = \frac{\bar{G}_{11}(z)}{1 - (\epsilon_i - \Sigma_{11}(z))\bar{G}_{11}(z)} \quad (35)$$

and

$$\bar{G}_{11}(z) = \int d\epsilon \frac{\rho_0(\epsilon)}{z - \Sigma_{11}(z) - \epsilon}; \quad (36)$$

$\rho_0(\epsilon)$ is the host metal density of states. Here we collect the analytical expressions for the Green's functions for three different ρ_0 functions.

(1) For the ellipsoidal density of states we have

$$\rho^0(E) = \frac{2}{\pi w^2} \sqrt{w^2 - E^2} \Theta(w^2 - E^2) \quad (37)$$

Here w is a half-width of the band; $\Theta(x) = 1$ for $x > 0$ and for $x < 0$. Integral (36) can easily be evaluated and we find

$$\bar{G}_{11}(z) = \frac{2}{w^2} \left(z + \mu - \Sigma_{11}(z) - \sqrt{(z + \mu - \Sigma_{11}(z))^2 + w^2} \right). \quad (38)$$

The conditionally averaged function (35) takes the following simple form

$$G_{11}^i(z) = \frac{1}{-\epsilon_i + z + \mu - \bar{G}_{11}(z)w^2/4}. \quad (39)$$

The self-energy $\Sigma_{11}(z)$ is determined by the cubic equation and can in principle be also calculated analytically.

(2) The lorentzian DOS obeys

$$\rho_0(\epsilon) = \frac{1}{\pi} \frac{w}{\epsilon^2 + w^2}. \quad (40)$$

Simple integrations lead to

$$\bar{G}_{11}(z) = (z - \Sigma_{11}(z) + \mu + iw \operatorname{sgn} \operatorname{Im} z)^{-1}, \quad (41)$$

$$G_{11}^i(z) = (z - \epsilon_i + \mu + iw \operatorname{sgn} \operatorname{Im} z)^{-1}. \quad (42)$$

CPA condition (19) can now be used to find the expression for Σ_{11} . For the $A_{1-x}B_x$ alloy it reads

$$\Sigma_{11}(z) = \mu + \langle \epsilon_i \rangle + \frac{x(1-x)(\epsilon_B - \epsilon_A)^2}{z + \mu + iw \operatorname{sgn} \operatorname{Im} z - x\epsilon_A - (1-x)\epsilon_B}. \quad (43)$$

(3) Concerning the DOS of the square lattice we make the following remarks.

The above two forms of the DOS have been widely used to simulate the DOS of the three-dimensional lattice. In view of the quasi-two-dimensional character of copper oxide superconductors and of several organic superconductors it may be instructive to study the density of states of a two-dimensional lattice. For free particles the DOS is known to be constant in 2 dimensions. On the contrary, it possesses a characteristic logarithmic singularity for the square lattice. With the help of eq. (3) the following exact representation of the DOS for the square lattice can be obtained

$$\rho_0(\epsilon) = N^{-1} \sum \delta(\epsilon + 2t(\cos k_x a + \cos k_y a)). \quad (44)$$

The alloy Green's function is expressed in terms of the elliptic integral $K(k)$ [15] as

$$G_{11}(z) = \frac{2}{\pi k} K(k), \quad k = (z + \mu - \Sigma_{11}(z))/2t. \quad (45)$$

The half-band-width is given now by $w = 4t$.

4.2. Analytical results for T_c

4.2.1. Solution for BCS model

The characteristic feature of the BCS model is the existence of the energy cut-off $\omega_0 \ll \mu, w$. In such a situation it is enough to evaluate the (in the interval of $2\omega_0$ around the Fermi level slowly varying) Green's functions in eq. (34) at the Fermi energy $\omega = z = i0$. One gets

$$T_c = 1.13\omega_0 e^{-1/\lambda_{\text{eff}}} \quad (46)$$

with the effective attraction parameter $\lambda_{\text{eff}} = \langle U_i \rho_i^2(0) / \rho(0) \rangle$. Here $\rho_i(0)$ and $\rho(0)$ denote the average and conditionally averaged alloy densities of states at the Fermi energy given by the imaginary parts of the Green's functions (35) and (36), respectively. The general form (46) does not depend on the density of states. For the lorentzian DOS we get an expression previously given by Weinkauff and Zittartz [13]

$$\lambda_{\text{eff}} = \frac{w}{w^2 + x\epsilon_A^2 + (1-x)\epsilon_B^2} \times \left\{ (1-x)U_A \frac{\epsilon_B^2 + w^2}{\epsilon_A^2 + w^2} + xU_B \frac{\epsilon_A^2 + w^2}{\epsilon_B^2 + w^2} \right\}. \quad (47)$$

4.2.2. The model with short range nonretarded attraction

In our model with local pairing the interaction has no cut-off and the neglect of the energy dependence of the Green's functions is not legitimate. Calculation of T_c from eq. (34) is possible but very tedious because of the ω and z dependence of the order parameter Σ_{12} . We shall therefore neglect the frequency dependence of it, which is equivalent to the factorisation of the average in eq. (34) by using

$$\left\langle \frac{G_{11}^i(z) - G_{11}^{i*}(-z^*)}{\bar{G}_{11}(z) - \bar{G}_{11}^*(-z^*)} \right\rangle = 1. \quad (48)$$

Then equation (34) takes on the simpler form

$$\bar{\Sigma}_{12}(\omega) = - \left\langle \frac{U_i}{\pi} \int d\omega \operatorname{th} \left(\frac{\beta\omega}{2} \right) \operatorname{Im} \left(\frac{G_{11}^i(\omega)}{2\omega} \bar{\Sigma}_{12}(\omega) \right) \right\rangle, \quad (49)$$

which is equivalent to the result presented previously [7,8].

We use eq. (41), evaluate integrals by means of contour integration and get the following exact condition for T_c :

$$1 = \left\langle \frac{U_i}{\pi} \sum_{n=0}^{\infty} \frac{1}{2n+1} \frac{(2n+1)\pi k T_c + w}{[(2n+1)\pi k T_c + w]^2 + (\epsilon_i - \mu)^2} \right\rangle. \quad (50)$$

This can be summed and expressed in terms of the di-gamma functions Ψ of complex argument [16] as

$$1 = \left\langle \frac{U_i}{\pi} \left\{ \operatorname{Re} \left[\frac{1}{w - \epsilon_i} \Psi \left(\frac{1}{2} + \frac{w}{2\pi T_c} + i \frac{\epsilon_i}{2\pi T_c} \right) \right] - \frac{w}{w^2 + \epsilon_i^2} \Psi \left(\frac{1}{2} \right) \right\} \right\rangle. \quad (51)$$

Noting that $\Psi(\frac{1}{2}) = -\gamma - 2\ln 2$, where $\gamma \cong 0.577$ is the Euler constant, and that asymptotically the function $\Psi(z) \cong \ln(z)$, we get an approximate expression for T_c :

$$T_c = \frac{2e^\gamma}{\pi} W_{\text{eff}} e^{-1/\lambda_{\text{eff}}}, \quad (52)$$

with effective attraction $\lambda_{\text{eff}} = \langle \rho_0(e_i) U_i \rangle$ and effective band width

$$W_{\text{eff}} = \exp \left\{ \left\langle U_i \rho_0(e_i) \left[\ln \sqrt{\frac{w}{\pi \rho_0(e_i)}} - \frac{e_i}{w} \operatorname{arctg} \frac{e_i}{w} \right] \frac{1}{\lambda_{\text{eff}}} \right\} \right\}. \quad (53)$$

Here, as usual $\langle O_i \rangle = (1-x)O_A + xO_B$; $\rho_0(e_i)$ is given by eq. (40) and for simplicity we have denoted $\epsilon_i - \mu$ by e_i . The concentration dependence of T_c is contained in e_i . At Fermi energy $e_i = 0$ and the argument of ρ_0 is zero. For a pure system with $\epsilon_A = \epsilon_B = 0$, $U_A = U_B = U$, $\lambda_{\text{eff}} = \rho_0(\mu)U$ and we recover the usual BCS-type solution with n dependent "cut-off" W_{eff} and λ_{eff} . In the clean limit, for the lorentzian density of states and at zero temperature eq. (13) can be evaluated exactly and one gets

$$n - 1 = \frac{2}{\pi} \operatorname{arctg} \frac{\mu}{w}.$$

In the $n \rightarrow 0$ limit we find from eqs. (52) and (53) the n dependence of T_c in the form

$$T_c \propto \frac{1}{n} \exp \left(- \frac{1-n}{n} \right) \exp \left(- \frac{4}{\pi w U n^2} \right).$$

Calculation of the zero temperature gap parameter $\bar{\Sigma}_{12}$ would be much more involved for an alloy because the order parameter Σ_{12} does depend on frequency ω through the renormalisation function $Z(\omega)$ even when $\bar{\Sigma}_{12}$ is constant. $Z(\omega)$ is defined by eq. (21); explicitly

$$Z(\omega) = \frac{2\omega}{2\omega + \Sigma_{11}^*(-\omega^*) - \Sigma_{11}(\omega)}. \quad (54)$$

$Z(\omega)$ is known to play an important role in the strong-coupling theory [11,17]. Here it results in the process of averaging. In the CPA we replace the real disordered system by the effective one described by the complex effective hamiltonian (here complex self-energies $\Sigma_{11}(\omega)$ and $\Sigma_{12}(\omega)$). The imaginary part of the self-energies has the interpretation of inverse lifetime of the particles. This introduces dynamical (ω -dependence) features into the problem which should affect the electromagnetic properties of the superconductors.

For the lorentzian DOS the function $Z(\omega)$ can be easily calculated. In fig. 1 we have shown plots of real and imaginary parts of $Z(\omega)$ for the present model and also for a square-lattice DOS. We can see the strong frequency dependence of both real (solid curves) and imaginary (broken curves) parts of $A(\omega)$ around the Fermi energy (zero of energy in these figures).

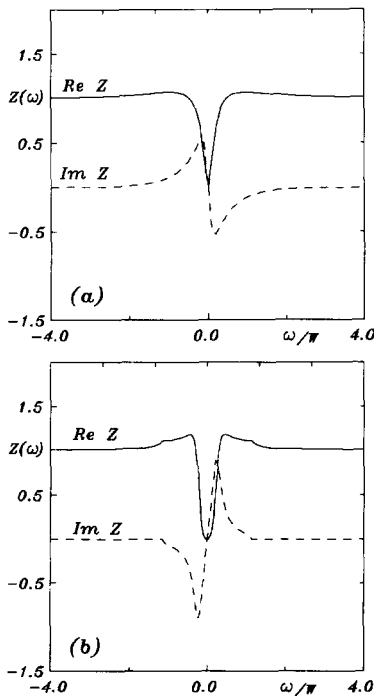


Fig. 1. The wave function renormalisation parameter $Z(\omega)$ (eq. 52) as a function of frequency for lorentzian host metal density of states (a) and square lattice DOS defined in eq. (43) (b). Note the strong frequency dependence of $Z(\omega)$ in the large part of the band. The alloy parameters are $x=0.5$, $\delta_0=0.45w$, $U=0.225w$ for both (a) and (b).

4.3. Numerical results and discussion

For numerical purposes we measure all energies and temperatures in units of the half band width w . An important parameter characterising the scattering properties of an alloy is the difference between unrenormalised energy levels $\delta_0 = \epsilon_A^0 - \epsilon_B^0$.

4.3.1. The metal-insulator transition

The (attractive) interaction between electrons leads to the formation of Cooper pairs but also to the renormalisation of the single particle energies via the Hartree term (8). This is an important factor leading to the appearance of the metal-insulator (M-I) transition when we vary the interaction parameters U_i , $i=A, B$. (when $U_A = U_B$ then the common value is denoted by U). We detect the M-I transition by observing the appearance of the gap in a single particle density of states $\rho(E)$ at the Fermi energy $E = E_F$. To calculate $\rho(E)$ from the imaginary part of the Green's function we have solved the system of eqs. (33) and (36) with corresponding host metal density of states $\rho_0(E)$, see eq. (37) or (44), and taking into account the renormalisation of the "atomic" levels ϵ_A and ϵ_B as expressed by eqs. (8), (30), (31) and (35). In figs. 2(a) and (b) we illustrate the renormalisation by plotting the difference $\delta = \epsilon_A - \epsilon_B$ as a function of concentration x for various values of the bare difference $\delta_0 = \epsilon_A^0 - \epsilon_B^0$. The effect is weak for small values of δ_0 and U (fig. 2(a)) increasing with the increase of both parameters. Note the difference between curves corresponding to positive and negative values of δ_0 which has an important influence on the metal-insulator (M-I) phase diagram. The phase diagram is shown in fig. 2(c) in the (δ_0, x) plane for $U=0.4w$. The metallic phase exists between the curves shown. Below the bottom curve and above the upper one the system is insulating. For a specific alloy (given value of δ_0) the model shows two transitions from insulator to metal, at low x and M-I at high x for positive δ_0 and even more consecutive transitions for negative δ_0 . Similar calculations have been presented in refs. [7] and [8], but the analysis of the M-I transition in ref. [7] was limited to positive δ_0 . In ref. [8] the phase diagram is shown on the (δ, x) plane. The phase diagram in our model does not depend on the form of the density of states.

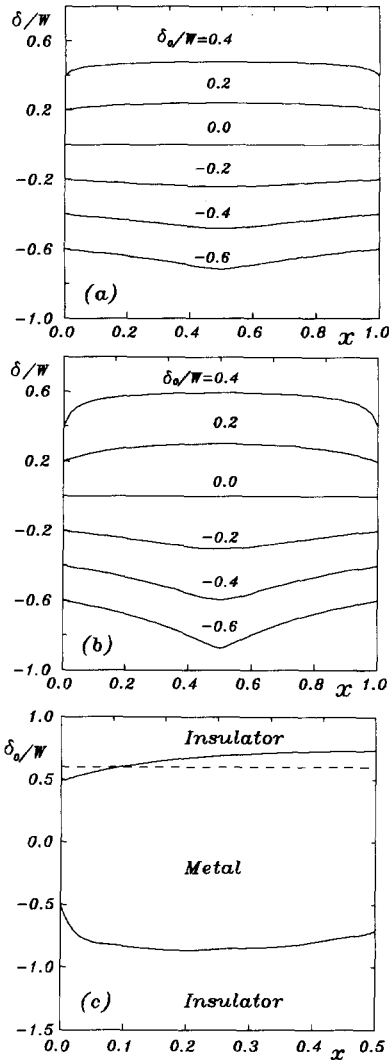


Fig. 2. The renormalised scattering potential parameter δ as a function of concentration x for a number of bare values δ_0 and $U=0.2w$ (a), and $U=0.4w$ (b). Figure (c) shows the regions of metallic and insulating phases on the δ_0, x plane for $U=0.4w$. Note the difference between $\delta_0 > 0$ and $\delta_0 < 0$ cases, connected with the Hartree term in eq. (8). These results do not depend on the density of states used.

Some additional insight into the system properties can be obtained by looking at the values of the DOS at the Fermi energy for different concentrations x . These are shown in fig. 3(a) for a semielliptic host metal DOS and in fig. 3(b) for a square lattice DOS for two values $\delta_0=0.6w$ and $-0.6w$ and $U=0.4w$. The difference between positive and negative values

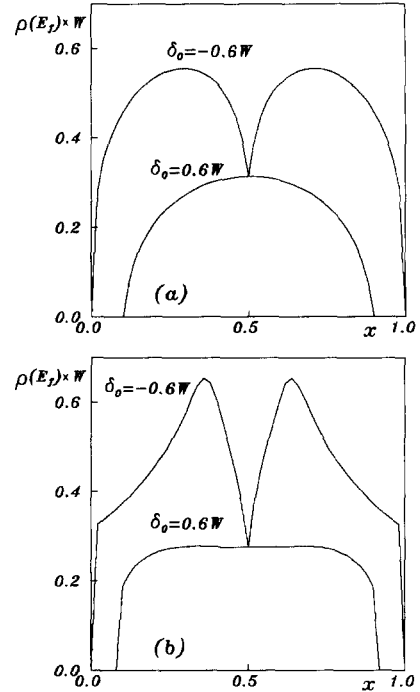


Fig. 3. The density of states at the Fermi energy plotted as a function of alloy composition for $U=0.4w$ and two values $\delta_0=0.6w$ and $-0.6w$, and a three-dimensional system with semielliptic DOS (a) and two-dimensional square lattice DOS (b). The value of $\rho(E_F)$ does not depend the sign of δ_0 for $x=0.5$ for symmetry reasons. The difference between $\rho(E_F)$ for $\delta_0 > 0$ and $\delta_0 < 0$ is mainly responsible for the differences noted in fig. 2.

of δ_0 is connected with renormalisation of single particle energies by the Hartree-Fock term $U_i \langle n_i \rangle$ in eq. (8). These in turn are responsible for the asymmetries in the phase diagram.

4.3.2. Superconducting critical temperature

In fig. 4 we show the dependence of the superconducting transition temperature on the concentration x for various strengths of the interaction parameter $U/w=0.3; 0.4; 0.5$ for an alloy with $\delta_0=0.6w$ (fig. 4(a)) and $\delta_0=-0.6w$ (fig. 4(b)). Note that T_c first increases (fig. 4(a)) with increasing U ($U=0.3w$, $U=0.4w$) and then decreases for $U=0.5w$ and larger values for $\delta_0 > 0$ but it increases monotonically (except for $x=0.5$) in the same range of attraction U for $\delta_0 < 0$. T_c has a maximum for half filled band (remember $n=2x$ in our model) when $\delta_0 > 0$ and it possesses a deep minimum at $x=0.5$ for $\delta_0 < 0$. This can

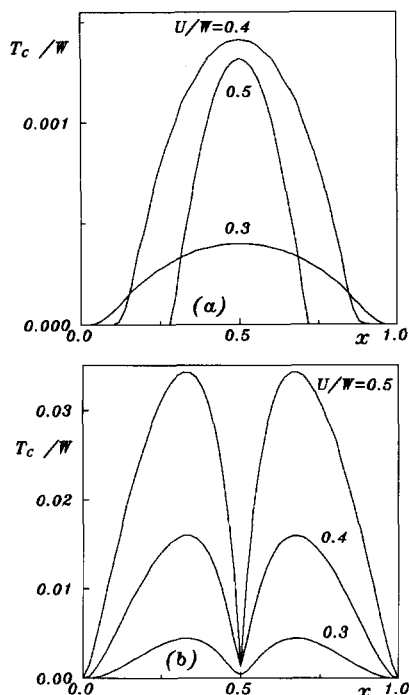


Fig. 4. The superconducting transition temperature as a function of alloy concentration (or carrier density $n=2x$) for a three-dimensional system, with various strengths of the on-site attraction U as indicated and $\delta_0=0.6w$ (a), and $\delta_0=-0.6w$ (b).

be simply explained by the behaviour of the density of states at the Fermi energy. Although our model does not imply any energy cut-off as in BCS theory, the structure of eq. (34) makes implicit that the density of states at E_F is the leading factor quantifying T_c . Figure 5 shows analogous results for a two-dimensional system. The overall behaviour is similar. The maximal value of the transition temperature is somewhat higher and the slopes of the curves for $x \rightarrow 0$ or 1 are different from the three-dimensional case.

In fig. 6 we show the plot of $T_c(x, \delta_0)$ for the $A_{1-x}B_x$ alloy with different interaction parameters $U_A=0.5w$ and $U_B=0.2w$. For negative δ_0 the T_c takes on appreciable values for $x \leq 0.5$. It follows from this figure that the functional dependence of T_c on the carrier concentration ($n=2x$) depends quite strongly on the alloy under consideration (δ_0, U_i).

Similar questions have been addressed previously [6,8]. Our condition (34) for the gap parameter $\tilde{\Sigma}_{12}(z)$ reduces to that presented in the cited works after additional factorisation of averages as ex-

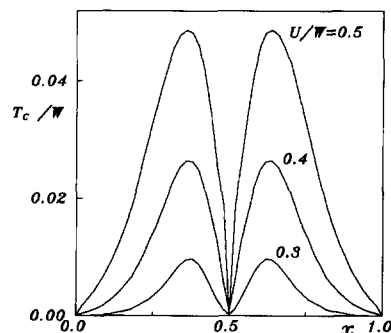


Fig. 5. T_c vs. n for a two-dimensional alloy with $\delta_0=-0.6w$ and for a few values of U/w as indicated. Note the slight increase of the maximal value of T_c and differences on the slopes of curves for $x \rightarrow 0$ and $x \rightarrow 1$ in comparison to the three-dimensional case.

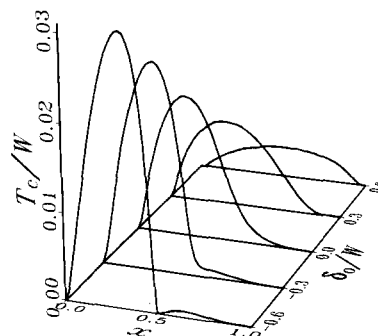


Fig. 6. Concentration dependence of T_c for a number of δ_0 values of the three-dimensional alloy with $U_A=0.5w$ and $U_B=0.2w$. The different values of U for the A and B components break the particle-hole symmetry and makes $T_c(x) \neq T_c(1-x)$ even in the system with no single particle scattering ($\delta_0=0$).

pressed in eq. (48). Such an approximation makes the gap parameter frequency independent and changes the dependence of T_c on x or n and U .

5. Final remarks

In the present work we have considered the weak coupling limit of the model (1) (i.e. $|U| < 2zt$). In the opposite large $|U|$ limit ($|U| \gg t$; preformed local pair regime) the model (1) can be reduced to that of the hard core charged Bose gas on a lattice in random chemical potential (see eq. (5) in ref. [5]). It is clear that as far as superconductivity is concerned the problem is equivalent to the dirty boson

problem whereas for the charge density wave (CDW) the problem is equivalent to that of antiferromagnets in random magnetic field. The effects of disorder on the stability of singlet superconductivity (SS) phase and the critical temperature in this case have been considered for two types of random site energy distribution:

(1) the two delta distribution with energies centered at $\pm E_0$ and

(2) the square distribution of width E_0 .

For the case (1) and $n=1$ increasing disorder suppresses SS if $2E_0/J_0 \geq 1$, where $J_0 = z 2t^2/|U|$ and z is the coordination number. An analysis of SS and CDW orderings also shows that increasing disorder stronger suppresses CDW than SS and that there exists a possibility of disorder induced superconductivity. It would be of interest to extend the analysis of the present paper to include the intersite Coulomb interaction to study the CDW ordering and mutual competition of CDW and SS. We should also stress that such an extension is necessary as far as a comparison with experiments on doped BaBiO_3 is concerned.

Here we have concentrated on the calculation of T_c of an superconducting alloy described by a negative U Hubbard model by treating attractive interactions in the broken symmetry Hartree–Fock approximation and disorder in CPA. The model describes the metal–insulator transition for high enough values of the interaction parameter U . When supplemented with the above mentioned intersite interaction it should describe the superconducting properties of $\text{BaPb}_{1-x}\text{Bi}_x\text{O}_3$ and possibly some of the high-temperature superconducting oxides with disorder introduced into the CuO planes.

The frequency dependence of the gap parameter is expected to play an important role in understanding electromagnetic properties of a superconductivity as e.g. the various features “inside” the gap in tunneling spectra. This problem is under investigation.

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