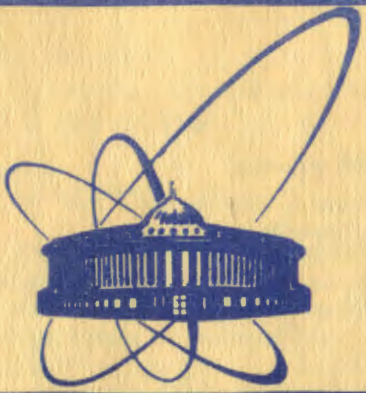

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SUPERCONDUCTIVITY IN A RANDOM LATTICE

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1. INTRODUCTION

Superconducting transition metal alloys of the type A_xB_{1-x} are characterized by a marked concentration dependence of the critical temperature $T_c(x)$ [1]. In such materials the d-electrons of narrow bands are responsible for superconductivity. The lattice sites are chemically inequivalent because they are randomly occupied by different kinds of atoms. Thus, T_c must be calculated by configurational averaging over a nonperiodic system, yielding an effective medium.

First treatments of disordered superconductors have been given for the "dirty" [2] and dilute alloy [3] cases. In the last years the coherent potential approximation (CPA) was used [4,5,6] to describe concentrated (nonmagnetic, weak-coupling) superconducting alloys on the basis of the lattice model.

$$\hat{H}' = \sum_{i\sigma} \epsilon_i c^+_{i\sigma} c_{i\sigma} + \sum_{\substack{ij\sigma \\ (i\neq j)}} t_{ij} c^+_{i\sigma} c_{j\sigma} - \sum (\Delta_i c^+_{i\uparrow} c^+_{i\downarrow} + \Delta^*_i c_{i\downarrow} c_{i\uparrow}) , \qquad (1)$$

where

$$\Delta_i = \lambda_i \langle\langle c_{i\downarrow} c_{i\uparrow} \rangle\rangle_{c,i} . \qquad (2)$$

Here the atomic energy ϵ_i, the hopping integrals t_{ij}, and the order parameter Δ_i assumed local are varying owing to the atomic disorder; $\lambda_i > 0$ is the random coupling parameter. The symbol $\langle \ldots \rangle$ means the thermal average; $\langle \ldots \rangle_{c,i}$ indicates the average over all atoms except the atom at site i. While t_{ij} and Δ_i are presumed to be nonrandom in ref. [4], spatial variations of the order parameter are taken into account in refs. [5,6]. Off-diagonal randomness (ODR), concerning t_{ij} in the multiplicative limit, was studied [6] in the framework of the CPA, too. In the presence of addive ODR but at constant order parameter, T_c and the gap were calculated [7] within the ODCPA scheme given in ref. [8].

The pairing term in (1) corresponds to the Hartree-Fock approximation of the BCS theory. Moreover, superconductivity can be derived from the fundamental fermion interaction by the functional integral technique. Such a procedure was

performed for pure superconductors [9-11]. The functional integral method (cf. ref. [12]) allows one to introduce collective quantum fields in a very natural way.

In this paper the functional integral formalism is applied to substitutionally discordered superconducting systems (Section 2). Including additive ODR, in Section 3 we evaluate T_c-formulae at constant and variable order parameters, respectively.

2. FUNCTIONAL INTEGRAL APPROACH

Consider a compositionally disordered superconductor for an arbitrary configuration of the atoms in an otherwise perfect lattice. At nonzero temperature $T=\beta^{-1}$ the random action reads

$$S=\int_0^\beta L(\tau)\,d\tau=\int_0^\beta d\tau\sum_{i\sigma}\bar{c}_{i\sigma}(\tau)\partial_\tau c_{i\sigma}(\tau)-\int_0^\beta H(\tau)\,d\tau \tag{3}$$

with L being the Lagrangian. The "time"-dependent tight-binding Hamiltonian is assumed to be of the form

$$H(\tau)=\sum_{i\sigma}\epsilon_i\,\bar{c}_{i\sigma}(\tau)c_{i\sigma}(\tau)+\sum_{\substack{ij\sigma\\(i\neq j)}}t_{ij}\,\bar{c}_{i\sigma}(\tau)c_{j\sigma}(\tau)-$$

$$-\sum_i\lambda_i\,\bar{c}_{i\uparrow}(\tau)\bar{c}_{i\downarrow}(\tau)c_{i\downarrow}(\tau)c_{i\uparrow}(\tau)\equiv H_V(\tau)+H_\lambda(\tau), \tag{4}$$

where ϵ_i, t_{ij} and λ_i are random parameters. The fundamental interaction part H_λ involves only local coupling. The generating functional Z for the fermion Green functions can be expressed by a path integral over anticommuting (Grassmann) variables as (cf. refs. [11,12])

$$Z[\bar{\eta},\eta]=\mathcal{N}\int D\bar{c}Dc\,e^{S[\bar{c},c]+\bar{c}\eta+\bar{\eta}c} \tag{5}$$

with the definitions (3), (4) and the abbreviation

$$\bar{c}\eta+\bar{\eta}c=\int_0^\beta d\tau\sum_{i\sigma}(\bar{c}_{i\sigma}(\tau)\eta_{i\sigma}(\tau)+\bar{\eta}_{i\sigma}(\tau)c_{i\sigma}(\tau)). \tag{6}$$

The normalization factor $\mathcal{N}$ is determined without external sources by setting $Z[0,0]=1$.

Taking into account that the c's in (5) are c-numbers, one can linearize the exponential of the quadratic interaction H_λ by the identity (with an irrelevant factor $\mathcal{N}_1$)

$$e^{\int_0^\beta d\tau \sum_i \lambda_i \bar{c}_{i\uparrow}(\tau)\bar{c}_{i\downarrow}(\tau)c_{i\downarrow}(\tau)c_{i\uparrow}(\tau)} \equiv e^{\lambda \bar{c}_\uparrow \bar{c}_\downarrow c_\downarrow c_\uparrow} =$$

$$= \mathcal{N}_1 \int D\Delta^* D\Delta\, e^{-\frac{1}{\lambda}|\Delta|^2 + \bar{c}_\uparrow \bar{c}_\downarrow \Delta + \Delta^* c_\downarrow c_\uparrow} . \qquad (7)$$

Here Δ represents the set of space- and "time"-dependent Bose (local pair) fields $\Delta_i(\tau)$. Then the generating functional (5) becomes

$$Z[\bar{\eta},\eta] = \mathcal{N}_2 \int D\bar{c}\, Dc\, D\Delta^* D\Delta\, e^{S_a[\bar{c},c;\Delta^*,\Delta] + \bar{c}\eta + \bar{\eta}c} \qquad (8)$$

with the augmented action (doublet notation $\bar{\psi} = (\bar{c}_\uparrow, c_\downarrow)$ and $\psi = \begin{pmatrix} c_\uparrow \\ \bar{c}_\downarrow \end{pmatrix}$)

$$S_a[\bar{c},c;\Delta^*,\Delta] = \bar{\psi} \begin{pmatrix} \partial_\tau - [H_V] & \Delta \\ \Delta^* & \partial_\tau + [H_V] \end{pmatrix} \psi - \frac{1}{\lambda}|\Delta|^2 . \qquad (9)$$

In view of (9) it is convenient to introduce the propagator matrix G_Δ written explicitly as

$$\sum_m \begin{pmatrix} \partial_\tau \delta_{im} - [H_V]_{im} & \Delta_i(\tau)\delta_{im} \\ \Delta_i^*(\tau)\delta_{im} & \partial_\tau \delta_{im} + [H_V]_{im} \end{pmatrix} G_{\Delta_{mj}}(\tau,\tau') = \delta_{ij}\,\delta(\tau-\tau'), \qquad (10)$$

where $[H_V]_{ij} = \epsilon_i \delta_{ij} + t_{ij}(1-\delta_{ij})$. In the static limit, (10) reduces to the Gorkov equations for disordered systems, which can be also obtained directly from the Hamiltonian (1).

The integration over the fermion fields in (8) leads to (functional Gaussian transformation)

$$Z[\bar{\eta},\eta] = \mathcal{N}_2 \int D\Delta^* D\Delta\, e^{S_{col}[\Delta^*,\Delta] + \bar{\xi} G_\Delta \xi} \qquad (11)$$

including the collective action

$$S_{col}[\Delta^*,\Delta] = \mathrm{Tr}\,\mathrm{tr}\ln G_\Delta^{-1} - \frac{1}{\lambda}|\Delta|^2 . \qquad (12)$$

Here the notation $\bar{\xi} = (\bar{\eta}_\uparrow, \eta_\downarrow)$, $\xi = \begin{pmatrix} \eta_\uparrow \\ \bar{\eta}_\downarrow \end{pmatrix}$, and $\frac{1}{\lambda}|\Delta|^2 \equiv \int_0^\beta d\tau \sum_i \frac{1}{\lambda_i}\Delta_i^*(\tau)\Delta_i(\tau)$

has been used; the trace Tr refers to site and "time" variables, while tr is restricted to the 2x2 (spin) matrix. According to the least action principle $\frac{\delta S_{col}[\Delta^*,\Delta]}{\delta\Delta_i^*(\tau)}=0$ we obtain the equation of motion for the collective field as

$$\Delta_i(\tau)=\lambda_i G^{12}_{\Delta ii}(\tau,\tau+0) \tag{13}$$

with $G^{12}_{\Delta}=\mathrm{tr}\,G_{\Delta}\begin{pmatrix}0&0\\1&0\end{pmatrix}$

Let us now rewrite the inverse Green function G_{Δ}^{-1} so that

$$\mathrm{Tr\,tr}\ln G_{\Delta}^{-1}=\mathrm{Tr\,tr}\ln G^{-1}+\mathrm{Tr\,tr}\ln\{1+G\begin{pmatrix}0&\Delta\\\Delta^*&0\end{pmatrix}\}, \tag{14}$$

where $G\equiv G_{\Delta=0}$ denotes the normal-state propagator. Thus, the collective action (12) can be expanded in powers of Δ as (the prime means including the term $\mathrm{Tr\,tr}\ln G^{-1}$ into the normalization)

$$S'_{col}[\Delta^*,\Delta]=\mathrm{Tr\,tr}\sum_{n=1}^{\infty}\frac{(-1)^{n+1}}{n}\{G\begin{pmatrix}0&\Delta\\\Delta^*&0\end{pmatrix}\}^n-\frac{1}{\lambda}|\Delta|^2=\sum_{n=1}^{\infty}S_n[\Delta^*,\Delta]-\frac{1}{\lambda}|\Delta|^2 \tag{15}$$

allowing the decomposition into the free and interacting parts:

$$S'_{col}[\Delta^*,\Delta]=S_{fr}[\Delta^*,\Delta]+S_{int}[\Delta^*,\Delta], \tag{16}$$

where

$$S_{fr}[\Delta^*,\Delta]=S_2[\Delta^*,\Delta]-\frac{1}{\lambda}|\Delta|^2, \tag{17}$$

$$S_{int}[\Delta^*,\Delta]=\sum_{n=2}^{\infty}S_{2n}[\Delta^*,\Delta]. \tag{18}$$

More explicitly, the free action (17) reads

$$S_{fr}[\Delta^*,\Delta]=-\int_0^{\beta}d\tau\,d\tau'\sum_{ij}\Delta_i^*(\tau)\left(G^{11}_{ij}(\tau,\tau')G^{22}_{ji}(\tau',\tau)+\frac{1}{\lambda_i}\delta_{ij}\,\delta(\tau-\tau')\right)\Delta_j(\tau') \tag{19}$$

expressed in terms of the elements of $G=\begin{pmatrix}G^{11}&0\\0&G^{22}\end{pmatrix}$. The corresponding Euler-Lagrange equation resulting from $\frac{\delta S_{fr}[\Delta^*,\Delta]}{\delta\Delta_i^*(\tau)}=0$ takes the form

$$\Delta_i(\tau) = -\lambda_i \int_0^\beta d\tau' \sum_j G_{ij}^{11}(\tau,\tau') G_{ji}^{22}(\tau',\tau) \Delta_j(\tau'). \qquad (20)$$

This relation coincides with the homogeneous Bethe-Salpeter equation in the presence of disorder.

3. DETERMINATION OF T_c VIA CONFIGURATIONAL AVERAGING

If the system is close to the critical region, all terms in the expansion (15) with $n > 2$ can be dropped in order to calculate the superconducting transition temperature T_c. Then we are left with the problem of averaging, in particular the equation (20), over all configurations of the lattice. The following treatment is based on the static approximation.

3.1. Anderson Case

The simplest case to find T_c consists in neglecting both the spatial and temporal fluctuations of the order parameter, i.e., in replacing

$$\Delta_i^{\{\nu\}}(\tau) \to \Delta, \qquad \lambda_i^{\nu} \to \bar{\lambda} = \langle \lambda_i^{\nu} \rangle_c, \qquad (21)$$

where the randomness is now explicitly labelled by $\nu(\{\nu\})$ for the site (whole lattice) occupation, $\langle \ldots \rangle_c$ denotes the configuration average. Then (19) can be rewritten by going over to Matsubara frequencies $z_n = i(2n+1)\pi T$ as

$$\langle S_{fr}^{\{\nu\}} \rangle_c = \frac{N}{T} \Delta^* \left[\frac{T}{N} \sum_n \langle \mathrm{Tr}\{ G^{11\{\nu\}}(z_n) G^{11\{\nu\}}(-z_n) \} \rangle_c - \frac{1}{\bar{\lambda}} \right] \Delta, \qquad (22)$$

where Tr means the trace only in the lattice space (N sites). By a Ward identity we get at arbitrary randomness in the normal scattering potential $\hat{V}^{\{\nu\}}$ ($\hat{H}_V^{\{\nu\}} = \hat{H}_0 + \hat{V}^{\{\nu\}}$):

$$\langle S_{fr}^{\{\nu\}} \rangle_c = \frac{N}{T} \Delta^* \left[\frac{T}{N} \sum_n \mathrm{Tr}\left\{ \frac{-\mathcal{G}(z_n) + \mathcal{G}(-z_n)}{2z_n} \right\} - \frac{1}{\bar{\lambda}} \right] \Delta = \frac{N}{T} \Delta^* M \Delta, \qquad (23)$$

where the averaged Green function is defined by

$$\mathcal{G}(z) = \langle G^{11\{\nu\}}(z) \rangle_c = (z - H_0 - \Sigma(z))^{-1}. \qquad (24)$$

By employing standard techniques [5,11] one obtains

$$M = \pi \rho(0)\, T \sum_n \frac{1}{|z_n|} - \frac{1}{\bar{\lambda}}, \qquad \rho(0) = -\frac{1}{\pi N} \mathrm{Tr}\, \mathcal{G}(+i0), \tag{25}$$

where M vanishes at the critical temperature

$$T_c = 1.13\, T_D \exp\{-\frac{1}{\bar{\lambda}\rho(0)}\}. \tag{26}$$

T_D is the Debye temperature. Hence the chemical potential of the pair field takes the form

$$M = \rho(0) \ln \frac{T_c}{T} \approx \rho(0)\,(1 - \frac{T_c}{T}). \tag{27}$$

The effect of disorder enters only through $\rho(0)$, i.e., the averaged density of states at the Fermi level $\mu = 0$ (Anderson theorem [2]). In the limit of the pure superconductor, (26) tends to the BCS result.

3.2. Random Order Parameter

Supposing spatial variations of the order parameter and taking the static limit of (13) and (20) we replace $\Delta_i^{\{\nu\}}(r)$ by

$$\begin{aligned} \Delta_i^\nu &= \lambda_i^\nu\, T \sum_n \langle i | \langle G_\Delta^{12\{\nu\}}(z_n) \rangle_{c,i}^\nu \, | i \rangle = \\ &= \lambda_i^\nu\, T \sum_n \langle i | G^{11\{\nu\}}(z_n) [\Delta^{\{\nu\}}] G^{11\{\nu\}}(-z_n) \rangle_{c,i}^\nu \, | i \rangle, \end{aligned} \tag{28}$$

where $[\Delta^{\{\nu\}}]_{ij} = \Delta_i^\nu \delta_{ij}$; the factor $e^{z_n 0^+}$ is omitted. Hereby, the complete randomness is reduced to the conditional average with respect to the site i. Let us assume additivity of the one-particle Hamiltonian by putting

$$\hat{H}_V^{\{\nu\}} = \hat{H}_0 + \sum_i \hat{V}_i^\nu \tag{29}$$

which involves ODR of the additive type, too. Then the partial averaging in (28) can be realized by

$$\langle G_\Delta^{12\{\nu\}}(z) \rangle_{c,i}^\nu = G_i^\nu(z)\,(\Delta(z) - \Delta_i(z) + [\Delta_i^\nu])\, G_i^\nu(-z) \tag{30}$$

leading to the total average

$$\langle\langle G_\Delta^{12\{\nu\}}(z) \rangle_{c,i}^\nu \rangle_c = \mathcal{G}(z)\, \Delta(z)\, \mathcal{G}(-z), \tag{31}$$

where

$$G_i^\nu(z) = \mathcal{G}(z) + \mathcal{G}(z)\, T_i^\nu(z)\, \mathcal{G}(z). \tag{32}$$

Here $\Delta(z)$ ($\Delta_i(z)$) denotes the anomalous self-energy (per site), and $[\Delta_i^\nu]_{mn}=\Delta_i^\nu \delta_{im}\delta_{mn}$. $\mathcal{G}$ is available from (24). T_i^ν is the single-site scattering matrix, having finite range in the lattice space in the presence of additive ODR. The conditionally averaged normal Green function G_i^ν satisfies the Ward-like relation

$$G_i^\nu(z)\,(2z-\Sigma(z)+\Sigma(-z)+\Sigma_i(z)-\Sigma_i(-z))\,G_i^\nu(z)=G_i^\nu(-z)-G_i^\nu(z)\,. \qquad (33)$$

Making the ansatz

$$\Delta_i(z)=\tilde{\Delta}(z)\left(\frac{-\Sigma_i(z)+\Sigma_i(-z)}{2z}\right)+\tilde{\Delta}_i(z) \qquad (34)$$

and correspondingly

$$\Delta(z)=\tilde{\Delta}(z)\left(\frac{2z-\Sigma(z)+\Sigma(-z)}{2z}\right) \qquad (35)$$

we find on comparing (30) and (31) the self-consistency condition

$$\langle G_i^\nu(z)\,\tilde{\Delta}_i(z)\,G_i^\nu(-z)\rangle_c=\langle G_i^\nu(z)\,[\Delta_i^\nu]\,G_i^\nu(-z)\rangle_c\,. \qquad (36)$$

This justifies to call $[\tilde{\Delta}_i(z)]_{mn}=\tilde{\Delta}(z)\delta_{im}\delta_{mn}$ the local coherent order parameter. Note that Δ_i as well as Σ_i are caused by an extended defect if additive ODR is taken into account. Combining (28), (30), (34) and (35) one can derive from (36) with the help of (33) the integral equation

$$\tilde{\Delta}(z)=T\sum_n \frac{K(z,z_n)}{z_n}\tilde{\Delta}(z_n)\,, \qquad (37)$$

where

$$K(z,z_n)=\frac{1}{2}\langle\lambda_i^\nu \frac{G_{ii}^\nu(z)-G_{ii}^\nu(-z)}{\mathcal{G}_{ii}(z)-\mathcal{G}_{ii}(-z)}(G_{ii}^\nu(-z_n)-G_{ii}^\nu(z_n))\rangle_c\,, \qquad (38)$$

and $G_{ii}^\nu \equiv \langle i|G_i^\nu|i\rangle$.

The equation (37) is solved approximately in the weak-coupling limit (cf. ref.[5]) by performing the Debye cutoff. One gets

$$T_c=1.13\,T_D\exp\{-\frac{\rho(0)}{\langle\lambda_i^\nu(\rho_i^\nu(0))^2\rangle_c}\} \qquad (39)$$

in terms of the partially averaged density of states

$$\rho_i^{\nu}(0) = -\frac{1}{\pi} \operatorname{Im} G_{ii}^{\nu}(+i0). \qquad (40)$$

In the case of only diagonal disorder (39) coincides with the T_c-formula in ref.[5] In contrast to ref.[5] the additive ODR included here brings out a momentum dependent self-energy $\Sigma(\vec{k}, z)$ entering via (24) and (32) into ρ and ρ_i^{ν}. The quantitative influence of different bandwidths of the components on T_c can be found on the basis of the ODCPA[8]. Numerical T_c-results have been reported in ref.[7] for the Anderson case.

Having introduced in the superconducting phase the functional integral over the complex order parameter space we restricted ourselves to the stationary point, i.e., to the classical solution of the collective quantum field. Indeed, we calculated T_c in the static limit by solving the scattering problem in the random potential.

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