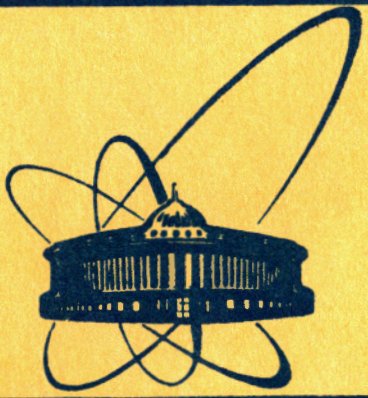

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LOCALIZATION VERSUS SUPERCONDUCTIVITY: COULOMB PSEUDOPOTENTIAL ENHANCEMENT

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1. INTRODUCTION

Experimentally, one observes (see hints in [1-3]) for some high-T_c, A-15 and cluster compound superconductors an "universal" drop of the superconducting transition temperature T_c versus ϱ curves (ϱ : low-temperature resistivity in the normal state, e.g., ϱ (T=25K) for V_3Si [1]). This is regardless of how disorder was produced, e.g., by α-particle and neutron irradiation [1], or alloying [3].

Theoretically, there is some controversy to explain the disorder-induced degradation of T_c which can be attributed to the decrease in the electronic density of states (at the Fermi energy) and in the electron-phonon coupling strength λ^{ph} [1,3], or to the increase in the Coulomb pseudopotential μ^* [2,4]. The latter mechanism is associated with a time-retarded Coulomb repulsion originated from electron localization.

In the finite-size scaling approach of Anderson et al. [2] the resistivity appears in μ^* as a measure of disorder in the resulting McMillan formula [5] for T_c. By means of a systematic combination of the self-consistent Vollhardt-Wölfle theory [6] of localization with the strong-coupling treatment [7] of tight-binding superconductivity, the T_c depression via μ^* was confirmed [4] in the regime of incipient localization $k_F \ell \geq 2$ (k_F : Fermi momentum, ℓ : elastic mean free path).

In this paper we extend the scheme [4] to the near-critical re-

gion $k_F\ell < 2$ (at the metallic side of the Anderson transition) with the emphasis on the enhancement of μ^*.

2. COULOMB KERNEL AND AC CONDUCTIVITY

Aimed at the superconducting T_c, we start with configurationally averaged[4,7] Eliashberg-type equations in the linearized form

$$z(1-Z(z)) = -\int_{-\infty}^{\infty} d\omega_2 K^{ph}(\omega_2, z) \quad , \tag{1}$$

$$\Delta(z)Z(z) = \int_{-\infty}^{\infty} d\omega_2 \left[K^{ph}(\omega_2, z) - \tfrac{1}{2}\mu(\tilde{\omega}_2)\,\mathrm{th}\,\frac{\omega_2}{2T}\right] \mathrm{Re}\,\frac{\Delta(\omega_2^+)}{\omega_2} \quad , \tag{2}$$

which determine the renormalization Z and the effective gap Δ functions, where $z = \omega^+ = \omega + i0$ and $\tilde{\omega} = \omega Z(\omega^+)$. The phonon kernel K^{ph} given in [4,7] is based on a contact-type electron-phonon interaction. The frequency-dependent Coulomb kernel

$$\mu(\omega) = \frac{1}{\varrho(0)N} \overline{\sum_i U_i \varrho_i(0)\varrho_i(\omega)} \tag{3}$$

involves the Hubbard-type repulsion U_i at site i. Here, the averaging over disorder is indicated by an overbar, and N is the number of lattice sites. The weighted mean in (3) is taken at the Fermi level being the energy origin. The averaged density of states (per site, per spin) $\varrho(\omega) = \frac{1}{N}\overline{\sum_i \varrho_i(\omega)}$ and the local density of states $\varrho_i(\omega) = -\frac{1}{\pi}\mathrm{Im}\,G^o_{ii}(\omega^+)$ are related to the normal-state Green function $G^o(z) = (z - H^o)^{-1}$, where the Hamiltonian H^o has in Wannier representation the matrix elements $H^o_{ij} = \varepsilon_i\delta_{ij} + t_{ij}(1-\delta_{ij})$. To establish the type of disorder we assume the atomic potential ε_i to be random and restrict ourselves to nearest-neighbour hopping $t_{ij} = t$. For Gaussian disorder, i.e., $\overline{\varepsilon_i} = 0$ and $\overline{\varepsilon_i\varepsilon_j} = W^2\delta_{ij}$, there exists [8] a critical ratio $\left(\frac{W}{t}\right)_{cr}$ sufficient to localize all the electronic states on the Fermi surface.

Let us express the joint local density of states $\frac{1}{N}\overline{\sum_i \varrho_i(0)\varrho_i(\omega)}$, as a measure of localization, by the normal density-density response (dynamic susceptibility)

$$\chi(\vec{q}, z_m) = -\frac{T}{N}\overline{\sum_{ijn} G^o_{ij}(z_n + z_m)G^o_{ji}(z_n)}\, e^{-i\vec{q}(\vec{R}_i - \vec{R}_j)}, \tag{4}$$

where $z_m = i2m\pi T$ and $z_n = i(2n+1)\pi T$ denote the Bose and Fermi frequencies, resp., and $\vec{R}_i$ is the position vector at site i. Using the spectral representation of G^o one gets

$$\mathrm{Im}\,\frac{1}{N}\sum_{\vec{q}}\chi(\vec{q},\omega^+) = \frac{1}{2N}\int_{-\infty}^{\infty} d\omega_1 d\omega_2\, \mathrm{Im}\left(\frac{\mathrm{th}\,\frac{\omega_2}{2T} - \mathrm{th}\,\frac{\omega_1}{2T}}{\omega^+ + \omega_2 - \omega_1}\right)\overline{\sum_i \varrho_i(\omega_1)\varrho_i(\omega_2)}$$

$$\approx \frac{\pi\omega}{N}\overline{\sum_i \varrho_i(0)\varrho_i(\omega)}\,, \tag{5}$$

where the last step can be justified in the zero-temperature limit and for a smooth integrand [4].

For small ω and q we make the diffusion ansatz

$$\chi(\vec{q},\omega^+) = \varrho(0)\,\frac{D(\omega)q^2}{D(\omega)q^2 - i\omega} \tag{6}$$

for the propagator (4) in the particle-hole channel, where $D(\omega)$ represents the frequency-dependent diffusion coefficient. In the metallic regime near the Anderson transition for d=3 one can evaluate $D(\omega)$ self-consistently from the equation [6]

$$\frac{D(\omega)}{D_o} = 1 - \frac{3}{\pi k_F^2 \ell}\int_0^{q_{max}} dq\, \frac{q^2}{q^2 - \frac{i\omega}{D(\omega)}} \tag{7}$$

with the upper momentum cut-off chosen to be $q_{max} = \frac{\pi}{\ell}$. Note that $D(0) \to 0$ signals localization for strong disorder in contrast with the bare diffusion constant $D_o = \frac{1}{3}\ell v_F$ (v_F: Fermi velocity) in the weak-scattering limit. To carry out the $\vec{q}$-sum on the l.h.s. of (5) we take into account (6), an analogous pole in the particle-particle channel for large q (the $D(\omega)$'s in both channels coincide due to time-reversal invariance), and the nonsingular contribution to χ from large momenta. Then, by using (3) and (7) we obtain

$$\mu(\omega) = U\varrho(0)\left[2\,\mathrm{Re}\,\tilde{\sigma}^{-1}(\omega) - 1\right]. \tag{8}$$

In getting (8) we have assumed the following: (i) a uniform U, (ii) the modified Einstein relation $\tilde{\sigma}(\omega) \equiv \frac{\sigma(\omega)}{\sigma_0} = \frac{D(\omega)}{D_0}$ valid for small ω, where $\sigma_0 = e^2 \varrho(0) D_0$ stands for the dc conductivity in the weak-scattering regime, and (iii) a parabolic band (effective mass approximation), yielding $\varrho(0) = \frac{k_F^2}{2\pi^2 v_F}$.

In view of (7), the dimensionless ac conductivity $\tilde{\sigma}(\omega)$ satisfies the self-consistency equation

$$\tilde{\sigma}(\omega) = 1 - \frac{3}{(k_F l)^2} + \alpha \left(- \frac{i\omega\tau}{\tilde{\sigma}(\omega)} \right)^{\frac{1}{2}} \qquad (9)$$

under the condition $\left| \frac{\omega\tau}{\tilde{\sigma}(\omega)} \right| \ll 1$ with the electron relaxation time $\tau = \frac{l}{v_F}$, and $\alpha = \frac{\sqrt{3}}{2} \frac{3}{(k_F l)^2}$. As a consequence of (9) one finds both the static conductivity

$$\sigma(0) = \sigma_0 \left(1 - \frac{3}{(k_F l)^2} \right) \qquad (10)$$

and the dynamical behaviour, so that asymptotically

$$\tilde{\sigma}(\omega) = \frac{2}{3} (\omega_c \tau)^{\frac{1}{3}} + \alpha^{\frac{2}{3}} (-i\omega\tau)^{\frac{1}{3}}, \qquad \omega \gg \omega_c . \qquad (11)$$

The scaling region $\omega \gg \omega_c$ is characterized by the crossover frequency ω_c defined by $(\omega_c \tau)^{\frac{1}{3}} \equiv \tilde{\sigma}(0) = \frac{l}{\pi \xi}$ (ξ: correlation length). At the critical point $\omega_c = 0$, or equivalently $(k_F l)_{cr} = \sqrt{3}$ corresponding to $\left(\frac{W}{t}\right)_{cr} = 4.22$ /4/ for a half-filled band and a sc lattice, we have the solution

$$\tilde{\sigma}(\omega) = \left(\frac{3}{4}\right)^{\frac{1}{3}} (\omega\tau)^{\frac{1}{3}} \left(\frac{\sqrt{3}}{2} - \frac{i}{2} \right). \qquad (12)$$

On the other hand, one can rewrite (9) via $\tilde{\sigma}(\omega) = (-i\omega\tau)^{\frac{1}{3}} F(\omega)$ in terms of the scaling function $F(\omega)$ /9/ obeying

$$F(\omega) = \left(i \frac{\omega_c}{\omega} \right)^{\frac{1}{3}} + \alpha F^{-\frac{1}{2}}(\omega). \qquad (13)$$

The corresponding β-function is explicitly found to be

$$\beta[F(\omega)] = \frac{d \ln F}{d \ln \omega} = \frac{2}{3} \frac{\alpha - F^{3/2}}{\alpha + 2F^{3/2}} . \qquad (14)$$

The zero of β at $F_{cr} = \alpha^{2/3}$ corresponds to (12).

3. LOCALIZATION EFFECT ON μ^*

In principle, we have to determine the overall influence of localization on T_c. Here, we only treat how strong disorder affects the Coulomb interaction $\mu(\omega)$, but not the electronic density of states $\varrho(0)$ and/or the electron-phonon interaction inherent in K^{ph}. To solve the basic Eliashberg-type equations (1) and (2) analytically, we employ the two square-well approximation giving rise to the McMillan formula /5/

$$T_c = \frac{\omega_D}{1.45} \exp\left\{ - \frac{1.04 (1 + \lambda^{ph})}{\lambda^{ph} - \mu^* (1 + 0.62 \lambda^{ph})} \right\} \qquad (15)$$

with the Debye frequency ω_D and the electron-phonon coupling parameter λ^{ph}.

To calculate the Coulomb pseudopotential μ^* we distinguish between three cases in tending to the Anderson transition from the metallic side.

(a) Incipient localization /4/, $\omega_c > \omega_D$, $k_F l \geq 2$ (i.e., $E_F \tau \geq 1$): There becomes

$$\mu^* = \frac{\mu'}{1 + \mu' \ln \frac{E_F}{\omega_D} - (\mu' - \mu) \ln \frac{E_F \tau}{\sqrt{\omega_c \tau}}} \qquad (16)$$

where $\mu' = \mu \left(\frac{2}{\tilde{\sigma}(0)} - 1 \right)$ and $\mu = U\varrho(0)$. Note that (16) rests on assuming a step function for $\mu(\omega)$, namely $\mu(\omega) = \left\{ \mu', \frac{1}{2}(\mu' + \mu), \mu \right\}$ within the intervals $\left\{ 0 < |\omega| < \omega_c , \omega_c < |\omega| < \frac{1}{\tau} , \frac{1}{\tau} < |\omega| < E_F \right\}$, resp.; do not confuse $\mu(\omega)$ and μ, hereafter.

(b) Near-critical regime, $0 < \omega_c < \omega_D$, $\sqrt{3} < k_F l < 2$: We propose the simple relation

$$\mu^* = \frac{\mu_0}{1 + \mu_1 \ln \frac{E_F}{\omega_D}} , \qquad (17)$$

which was based on the frequency dependence $\mu(\omega) = \mu_0$ for $0 < \omega < \omega_D$ and $\mu(\omega) = \mu_1$ for $\omega_D < \omega < E_F$. There are some possibilities to fix μ_0 and μ_1. For example, at $\omega_c \neq 0$, one can choose $\mu_0 = \frac{1}{2}(\mu' + \mu(\omega_D(1+\lambda^{ph})))$ and $\mu_1 = \frac{1}{2}(\mu(\omega_D) + \mu)$.

(c) Critical point, $\omega_c = 0$, $(k_F l)_{cr} = \sqrt{3}$:

In this case the expression (17) for μ^* holds, too. Formally, one may put $\mu_0 = \frac{1}{\omega_D}\int_0^{\omega_D} d\omega\, \mu(\omega(1+\lambda^{ph}))$ which remains finite although the integrand becomes singular at $\omega = 0$ in view of (8) and (12). One gets $\mu_0 = \mu \cdot (3\, \mathrm{Re}\, \tilde{\sigma}^{-1}(\omega_D(1+\lambda^{ph})) - 1)$. The quantity μ_1 varies between $\mu(\omega_D)$ and $\mu(E_F) = \mu$, where the latter value follows from (8) and (12). Note that the Drude formula $\tilde{\sigma}^{-1}(\omega) = 1 - i\omega\tau$ yields the same limit for $\mu(E_F)$. By analogy with μ_0 we take the mean value $\mu_1^{I} = \frac{1}{E_F - \omega_D}\int_{\omega_D}^{E_F} d\omega\, \mu(\omega)$ $= \mu\left(3\, \mathrm{Re}\, \tilde{\sigma}^{-1}(E_F)\left(\frac{1 - (\frac{\omega_D}{E_F})^{2/3}}{1 - \frac{\omega_D}{E_F}}\right) - 1\right)$. Alternatively, we could approximate μ_1 by $\mu_1^{II} = \frac{1}{2}(\mu(\omega_D) + \mu)$; however, an arithmetic mean for μ_0 would go to infinity.

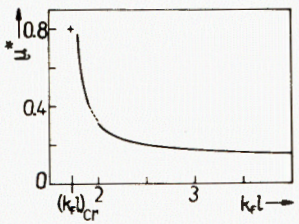

Fig. Coulomb pseudopotential μ^* affected by localization in dependence on the degree of disorder $k_F l$, $(k_F l)_{cr}$ refers to critical disorder. Parameters: $\mu = 0.3$, $\ln \frac{E_F}{\omega_D} = 4.5$, $\lambda^{ph} = 1$.

Now we turn to the numerical estimation of the Coulomb pseudopotential μ^*. The parameters are chosen to be $\mu = 0.3$, $\ln \frac{E_F}{\omega_D} = 4.5$, and $\lambda^{ph} = 1$, which may model the high-T_c superconductor $LuRh_4B_4$ /2/. The Figure shows the numerical results of μ^* calculated for $k_F l \geq 2$ from (16), and for $k_F l < 2$ from (17). In particular, at the critical point $(k_F l)_{cr} = \sqrt{3}$, one finds $\mu^* = 0.8$ resulting from μ_1^{I} (cf. case (c)). Taking into account μ_1^{II}, one would obtain $\mu^* = 0.4$ reflecting the high sensitivity of μ^* with respect to the approximation made. For weak

disorder, e.g., $k_F l = 4$ in the Figure, one arrives at the classical value $\mu^* = 0.15$. For comparison, $\mu^* = 0.1 - 0.17$ typifies pure transition metals /5/. The frequency dependence in $\mu(\omega)$ due to localization is responsible for the anomalous enhancement of μ^*. Without such a retardation effect, μ^* remains relatively small ($\mu^* = 0.22$ if $\mu \to \infty$).

According to (15) superconductivity ceases for $\mu^* = 0.62$ corresponding in our scheme to the resistivity $r = \sigma^{-1}(0) \approx 845\,\mu\Omega\,\mathrm{cm}$. From the experimental point of view, superconductivity may survive for high resistivity /1/. This disagreement may be due to the breakdown of the McMillan formula for large μ^* /3/. However, our $T_c(r)$ results for $k_F l \geq 2$ are in good agreement with experimental data on some high-T_c superconductors as demonstrated in /4/. As stated in /10/, without taking into account the Coulomb repulsion explicitly, a system which is Anderson localized in the normal state may become superconducting. To conclude, the correction of McMillan's formula near critical disorder must be connected with the localization effect on λ^{ph}.

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Коллей Е., Коллей В. E17-84-634

Локализация и сверхпроводимость:
усиление кулоновского псевдопотенциала

На основе самосогласованной теории андерсоновской локализации найдено зависящее от частоты кулоновское ядро уравнения типа Элиашберга для сильно разупорядоченного сверхпроводника. Получено возрастание кулоновского псевдопотенциала μ^*, приводящее к уменьшению критической температуры сверхпроводимости T_c в области металлической фазы вблизи точки перехода Андерсона.

Работа выполнена в Лаборатории теоретической физики ОИЯИ.

Сообщение Объединенного института ядерных исследований. Дубна 1984

Kolley E., Kolley W. E17-84-634

Localization versus Superconductivity:
Coulomb Pseudopotential Enhancement

The frequency-dependent Coulomb kernel of the Eliashberg-type equation for strongly disordered superconductors is found on the basis of the self-consistent theory of Anderson localization. The increase in the Coulomb pseudopotential μ^*, leading to the "universal" degradation of the superconducting transition temperature T_c, is evaluated in the metallic region near critical disorder.

The investigation has been performed at the Laboratory of Theoretical Physics, JINR.

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