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SPATIAL VARIATIONS OF ORDER PARAMETER NEAR ANDERSON IMPURITY IN SUPERCONDUCTORS

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1. INTRODUCTION.- Since the first attempt by Tzuzuki and Tsuneto /1/ several calculations have been performed of the spatial dependence of the order parameter \( \Delta(r) \) in superconductors containing a single magnetic impurity (see Schlottmann /2/ and references therein). For a nonmagnetic impurity \( \Delta(r) \) has been calculated by Fetter /3/ taking into account the nonresonant scattering of conduction electrons. The importance of resonant scattering, caused by transition metal impurities, for the decrease of \( T_c \) was first demonstrated by Zuckermann /4/ using the Anderson's model for localized states in metals /5/. The purpose of the present paper is to describe a calculation of \( \Delta(r) \) using the same model. The motivation for our work is the relaxation study on Al nuclei in Al-Mn alloys by Daugherty, et al. /6/. These authors have presented evidence for an anomalous broadening of the density of states below \( T_c \). In their alloys the average distance of the resonating nuclei from the impurities is of the order of 100 \( \text{Å} \) and thus one expects that short range variations of \( \Delta(r) \) could provide a possible explanation of the above broadening.

2. THEORY.- We employ the Hamiltonian of a BCS superconductor containing a single impurity at the origin:

\[
H = H_n - \int d^3r \left[ \Delta^0(r) \Psi_+(r) \Psi_0(r) + h.c. \right]
\]

where \( H_n \) is the Anderson Hamiltonian /5/ and \( \Delta(r) = g < \Psi_+(r) \Psi_0(r) > \) is the local parameter. Near \( T_c \) the anomalous average can be evaluated to first order in \( \Delta \) yielding

\[
\Delta(r) = g \int d^3r' \Delta(r') \beta \int_0^\beta dt < T_s \Psi_+(r,0) \Psi_0(r,0) \Psi_+(r',t) \Psi_0(r',t) > _n (2)
\]

where \( \beta = 1/T \) and the average of the time ordered operator product is to be taken over the states of \( n = H_n \). Explicit evaluation of this average bears certain similarities to the calculation of the depression of \( T_c \) in superconducting alloys by Sakurai /7,8/. Performing the angular average of the kernel of the gap equation, we obtain, from equations (1) and (2),

\[
\Delta(r) = g T \sum_{\epsilon} \int d^3r' \Delta(r') \left[ G_0(r-r',\epsilon) G_0(r-r',-\epsilon) + (2\zeta + 1) \frac{\Gamma}{\pi} \frac{G_0(r-r',\epsilon) G_k(r,\epsilon) G_k(r,\epsilon) G_0(r-r',\epsilon) + G_0(r-r',-\epsilon) G_k(r,\epsilon) G_0(r-r',\epsilon)}{\epsilon^2 - \epsilon_0^2} \right]
\]

where the summation over discrete frequencies \( \epsilon = (2n+1)\pi T \) involves a Debye-cutoff at \( |\epsilon| = \omega_0 \).

\[
\Gamma_{\epsilon_0,\epsilon} = \int d^3r' G_0(r',\epsilon_0) G_k(r',\epsilon_1) G_0(r',\epsilon_2) G_0(r',\epsilon_3) \Gamma_{\epsilon_1,\epsilon_2} \Gamma_{\epsilon_2,\epsilon_3} \Gamma_{\epsilon_3,\epsilon_0} (3)
\]

where the summation over discrete frequencies \( \epsilon = (2n+1)\pi T \) involves a Debye-cutoff at \( |\epsilon| = \omega_0 \).

\[
G_0(r,\epsilon) = G_k(r,\epsilon) G_0(r,\epsilon) G_0(r,\epsilon) G_0(r,\epsilon) \Gamma_{\epsilon_1,\epsilon_2} \Gamma_{\epsilon_2,\epsilon_3} \Gamma_{\epsilon_3,\epsilon_0} (3)
\]

\[
H = H_n - \int d^3r \left[ \Delta^0(r) \Psi_+(r) \Psi_0(r) + h.c. \right]
\]

where \( H_n \) is the Anderson Hamiltonian /5/ and \( \Delta(r) = g < \Psi_+(r) \Psi_0(r) > \) is the local parameter. Near \( T_c \) the anomalous average can be evaluated to first order in \( \Delta \) yielding

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\Delta(r) = g \int d^3r' \Delta(r') \beta \int_0^\beta dt < T_s \Psi_+(r,0) \Psi_0(r,0) \Psi_+(r',t) \Psi_0(r',t) > _n (2)
\]

where \( \beta = 1/T \) and the average of the time ordered operator product is to be taken over the states of \( n = H_n \). Explicit evaluation of this average bears certain similarities to the calculation of the depression of \( T_c \) in superconducting alloys by Sakurai /7,8/. Performing the angular average of the kernel of the gap equation, we obtain, from equations (1) and (2),

\[
\Delta(r) = g T \sum_{\epsilon} \int d^3r' \Delta(r') \left[ G_0(r-r',\epsilon) G_0(r-r',-\epsilon) + (2\zeta + 1) \frac{\Gamma}{\pi} \frac{G_0(r-r',\epsilon) G_k(r,\epsilon) G_k(r,\epsilon) G_0(r-r',\epsilon) + G_0(r-r',-\epsilon) G_k(r,\epsilon) G_0(r-r',\epsilon)}{\epsilon^2 - \epsilon_0^2} \right]
\]

where the summation over discrete frequencies \( \epsilon = (2n+1)\pi T \) involves a Debye-cutoff at \( |\epsilon| = \omega_0 \).

\[
\Gamma_{\epsilon_0,\epsilon} = \int d^3r' G_0(r',\epsilon_0) G_k(r',\epsilon_1) G_0(r',\epsilon_2) G_0(r',\epsilon_3) \Gamma_{\epsilon_1,\epsilon_2} \Gamma_{\epsilon_2,\epsilon_3} \Gamma_{\epsilon_3,\epsilon_0} (3)
\]

where the summation over discrete frequencies \( \epsilon = (2n+1)\pi T \) involves a Debye-cutoff at \( |\epsilon| = \omega_0 \).

\[
H = H_n - \int d^3r \left[ \Delta^0(r) \Psi_+(r) \Psi_0(r) + h.c. \right]
\]

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symbol $\Gamma_{++}^{\pm}(\varepsilon,\varepsilon')$ stands for the vertex part /7/ due to inelastic scattering of up and down spin electrons via the repulsive interaction $U$. For a symmetric Anderson model the $\varepsilon$-dependence of both $\Gamma_{++}^{\pm}$ and $G_0$ can be determined (for $\varepsilon$ and $T \ll$ Kondo temperature $T_K$) via the microscopic Fermi liquid theory /7,8,10/. Consequently for transition-metal impurities with $T_K$ large compared to $\omega_D$ the kernel of the integral equation (3) can be calculated as an expansion in $\omega_D/T_K$. To estimate the spatial variations in the vicinity of the impurity we iterate equation (3) by putting $A(r') = A$ and evaluate the kernel to the leading order in $\omega_D/T_K$. For distances such that $1 \ll k_F r \ll \varepsilon_F/\omega_D$ the $\varepsilon$-summations in equation (3) can be performed yielding

$$[\Delta(\tau) - \Delta_o]/\Delta_o = -2 \left(\frac{2\pi+1}{(2\pi)^2}\frac{\sin^2 k_F r}{(k_F^2 r)^2} + \frac{(2\pi+1)}{(k_F^2 r)^2} - \frac{2\pi}{(k_F^2 r)^2} \frac{\omega_D}{\omega_D} \right) \chi_{++}^{4+} \tag{4}$$

where $\chi_{++}^{4+}$ is the odd-part of the normalized d-electron susceptibility /10/. For Al-Mn alloy we put $\Gamma = 1.4 \times 10^4$ K, $\omega_D = 4 \times 10^2$ K and $\chi_{++}^{4+} \approx 10 /8/$. With these parameters the third term of equation (4), representing the inelastic scattering, turns out to be only about $15 \times 10^{-2}$ times the magnitude of the first resonant scattering term. For the nearest neighbor Al-alkaline ($k_F r_1 = 5$) equation (4) predicts $(\Delta(\tau) - \Delta_o)/\Delta_o = 1$ showing that resonant scattering leads to a strong change of the local order parameter in the vicinity of the Mn-impurity. This is in contrast with the calculations of the change of $T_c$ /7,8/ where the inelastic contribution is larger. In general, for alloys with $T_K$ large compared to $\omega_D$ (such as Fe group in Al) the inelastic contribution to equation (4) is small compared to the resonant contribution. It is interesting that Parvin and MacLaughlin /11/ recently found an evidence that Mn and V in Al produce a density of states broadening of about the same size. This independence of the impurity $T_K$ provides an additional argument to anticipate that short range variations of $\Delta(r)$ due to resonant scattering may be the mechanism of the broadening.

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