Growth in T_c of a superconductor in the instability region of a univalent state of Anderson impurities with local electron-phonon interaction

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(Submitted 30 July 1991)
Zh. Eksp. Teor. Fiz. **101**, 1005–1013 (March 1992)

The effect of a small concentration of Anderson impurities on the critical temperature T_c of a superconductivity transition is studied. The impurities are described by Anderson's Hamiltonian to which the interaction of electrons on the quasistationary level of an impurity with lattice vibrations is added. The region is studied where the univalent state is unstable, characterized by a strong anharmonicity of the lattice-atom vibrations near an impurity or of the impurity atoms proper. It is shown, within the framework of the Fermi-liquid theory, that T_c markedly grows even if the Coulomb repulsion of electrons on a local impurity level is infinitely strong.

1. INTRODUCTION

Models that predict high T_c values are of particular interst in connection with the problem of high-T_c superconductivity. Earlier it was shown[1–3] that even a small concentration of Anderson impurities in a metal can lead to a marked increase in T_c, provided that the electrons localized on the quasistationary levels of the impurities strongly interact with the vibrations of the impurities proper or their surrounding. The term "Anderson impurity" implies that the impurity is associated with a nondegenerate level which mixes, via single-particle interaction, with the electronic states in the broad conduction band of the metal. In addition, one must allow for the Coulomb repulsion of two electrons on this level. Thus, the system is described by the standard Anderson Hamiltonian to which the interaction of the electrons on the local level with the lattice vibrations is added.

An important feature of this model is the instability of the equilibrium positions of the oscillators associated with the impurity, when the electron-phonon coupling constant ξ becomes larger than a certain critical value ξ_c (see Refs. 4 and 5). In the adiabatic approximation (it is assumed that the lattice vibration frequency is much lower than all characteristic electron energies, including the width Γ of the quasistationary electron level of an impurity), this instability resembles a transformation of single-well adiabatic term into a double-well. The different valences of the impurity correspond to the two minima of this potential well. The dynamic behavior of the electron-phonon system is determined largely by the height of the potential barrier between these two states, which grows in the region where $\xi > \xi_c$ with ξ. The impurities have a different effect on the superconductivity of a metal in different dynamic modes. Several limiting cases have been discussed in Refs. 6 and 7.

Below we consider the region near the stability boundary for the univalent state, where $|\xi - \xi_c| \ll 1$. As shown earlier,[5,6] when ξ approaches ξ_c from below, the constant of effective attraction between electrons increases, and in the harmonic approximation it becomes infinite. However, for $|\xi - \xi_c| \ll 1$, the lattice vibrations related to the impurity are highly anharmonic, a feature that must be taken into account when calculating this constant. An important fact that makes a fairly meaningful solution of the given problem possible is the applicability of the adiabatic approximation for $|\xi - \xi_c| \ll 1$. Within this range the state of the impurity is characterized by the presence of fairly rapid valence fluctuations, while for $|\xi - \xi_c| \gtrsim 1$ the adiabatic approximation breaks down owing to the well-known infrared divergences in the response of electrons to slow quantum fluctuations of the system between two (degenerate) states.

The possibility of employing the adiabatic approximation for arbitrary values of the energy U of the Coulomb repulsion of the electrons localized on the impurity is also ensured by the fact that near the stability boundary of the univalent state on the impurity there is no localized magnetic moment (or it is small), in other words, the Kondo temperature T_K is high, so that $kT_K \sim \Gamma$. Thus, the adiabatic approximation is valid if the vibration frequency ω_0 is much lower than Γ, so that Γ is the lowest of the characteristic electron energies. This in turn permits, within the framework of the Fermi-liquid theory, all the quantities important for the problem under discussion to be expressed in terms of the DC susceptibilities of the impurity, which are known for arbitrary values of U from the exact solution of the Anderson model.[8,9]

This paper is built along the following lines. In Sec. 2 we derive all the relations needed for calculating T_c. In Sec. 3 we study the dynamics of anharmonic vibrations and numerically find T_c for two limiting cases, $U = 0$ and $U = \infty$.

2. AN EQUATION FOR T_c

The system's Hamiltonian is

$$H = \sum \varepsilon_{\mathbf{k}} n_{\mathbf{k}\sigma} + \sum \varepsilon n_{i\sigma} + \sum V \exp(i\mathbf{k}\mathbf{r}_i) d_{i\sigma}{}^{+} c_{\mathbf{k}\sigma} + \text{H.c.} + U \sum_i n_{i\sigma} n_{i-\sigma} + \alpha \sum q_i n_{i\sigma} + \sum \left(\frac{p_i{}^2}{2M} + \frac{M\omega_0{}^2 q_i{}^2}{2} \right). \tag{1}$$

The first four terms constitute Anderson's Hamiltonian, where $c^{+}_{\mathbf{k}\sigma}$, $c_{\mathbf{k}\sigma}$ and $d^{+}_{i\sigma}$, $d_{i\sigma}$ are, respectively, the creation and annihilation operators for electrons in the conduction band and on the local level of the ith impurity, $n_{i\sigma} = d^{+}_{i\sigma} d_{i\sigma}$, and $n_{\mathbf{k}\sigma} = c^{+}_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma}$. The other terms describe the vibrational degrees of freedom q_i, represented for simplicity by Einstein oscillators (one oscillator for each impurity), and the interaction of these with electrons.

0038-5646/92/030539-05$05.00

The temperature of the superconductivity transition can be determined from the linearized equation for the band gap[10]

$$\Delta(\omega)=-T_c\sum{}'\Gamma(\omega,\omega')[G_{\mathbf{k},\mathbf{k}'}(\omega')G_{-\mathbf{k},-\mathbf{k}'}(-\omega')]_{av}\Delta(\omega'), \tag{2}$$

where $[\cdots]_{\text{av}}$ stands for averaging over the positions of the impurities, and summation is carried out over the wave vectors $\mathbf{k}$ and $\mathbf{k}'$ and over the discrete frequencies $\omega'=2\pi(n+\frac{1}{2})T_c$. The vertex function consists of two parts: the BCS interaction in the metal and the vertex Γ_i caused by the scattering of electrons on impurites. It is also important to allow for this scattering (both elastic and inelastic) in the self-energy part of the electron Green function $G_{\mathbf{k},\mathbf{k}'}(\omega)$.

In the lowest perturbation-theory order in the Coulomb interaction U and the electron-phonon interaction we have

$$\Gamma_i(\omega,\omega')=|V|^4c|G_d^0(\omega)|^2|G_d^0(\omega')|^2[U+\alpha^2D(\omega-\omega')], \tag{3}$$

where c is the impurity concentration, $G_d^0(\omega)=(i\omega-\varepsilon+i\Gamma\operatorname{sign}\omega)^{-1}$ the unperturbed Green function of electrons on a quasistationary impurity level $\Gamma=\pi N(0)|V|^2$ wide, $N(0)$ the density of states of the electrons on the Fermi surface, and $D(\omega)$ the Green function of the oscillator q_i. The second term in (3) reflects the interaction of these electrons with lattice vibrations and leads to effective attraction between them for $|\omega-\omega'|\lesssim\omega_0$. When the attraction is sufficiently strong, even low concentrations of impurities may considerably increase T_c (see Refs. 1-3). To a great extent this is due to the presence of Γ_i of resonance factors $|G_d(\omega)|^2$ which are large for $\omega,\varepsilon\lesssim\Gamma$. For the same reason, when the repulsion U is predominant in (3), the impurities lead to a strong suppression of T_c, as is known from Ref. 11.

The perturbation-theory approach assumes that U is small compared to Γ. In many interesting cases, however, the situation is just the opposite, $U\gg\Gamma$, and perturbation-theory expansions in U are invalid. At the same time, the presence of an adiabatic parameter $\omega_0\ll\Gamma$ makes it possible, even when the electron-phonon interaction is strong (at least when $\xi\omega_0/\Gamma\ll1$, with $\xi=\alpha^2/M\omega_0^2\Gamma$), to limit oneself to lowest orders in the electron-phonon interaction, as is usually done when considering ordinary superconductors. Hence, instead of (3) we have

$$\Gamma_i(\omega,\omega')=c|V|^4|G_d(\omega)|^2|G_d(\omega')|^2[\Gamma_c(\omega,\omega')+\alpha^2|F(\omega,\omega')|^2D(\omega-\omega')], \tag{4}$$

where $\Gamma_c(\omega,\omega')$ is the total vertex of two-particle electron-phonon interaction in the Cooper channel, which includes the interaction U in all orders, and $F(\omega,\omega')$ the form factor determining the renormalization of the electron-phonon interaction vertex. Note that since for each impurity only the pair correlators of the oscillator coordinates q are included in $\Gamma_i(\omega,\omega')$, formula (4) is valid not only for a harmonic oscillator but also when the oscillator's potential energy has an arbitrary shape. This makes it possible to calculate T_c in the lattice's local instability range, where the lattice vibrations near impurities are highly anharmonic. It is assumed, of course, that the characteristic frequencies of motion in this potential are much lower than Γ, and Γ is the smallest energy parameter of the electronic subsystem. This occurs in the absence of a localized magnetic moment on the impurity or when this moment is low (the Kondo temperature $T_{\text{K}}\sim\Gamma$ is high).

It is not necessary to calculate $\Gamma_i(\omega,\omega')$ in the entire frequency range in order to find T_c. In the logarithmic approximation, within the framework of the BCS theory, it is sufficient to know the value of $\Gamma(0,0)$ and the frequency scales over which $\Gamma_c(\omega,\omega')$ and $D(\omega)$ vary in Eq. (4). Obviously, the width Γ of the quasistationary level serves as the scale for $\Gamma_c(\omega,\omega')$, and $D(\omega)$ decreases at the characteristic frequencies of the oscillator vibrations. The value of $\Gamma_c(0,0)$ can be expressed in terms of the DC spin and charge susceptibilities of the impurity by employing Ward identities. This has been done in Ref. 12 in the problem of suppressing superconductivity by magnetic impurities in the symmetric Anderson model. The result obtained there can easily be generalized to the asymmetric model (see the Appendix). Thus, we have

$$|G_d(0)|^4\Gamma_c(0,0)=(\chi_{sp}-\chi_{ch})\pi^2/\Gamma^2, \tag{5}$$

where χ_{sp} and χ_{ch} are the DC spin and charge susceptibilities of the impurity.

When $F(\omega,\omega')$ is calculated in the adiabatic approximation, the q_i can be interpreted as the static displacements of the coordinates of the oscillators, which lead to a shift in the energy ε in (1) by αq_i. Then the function $F(\omega,\omega')$ at $\omega=\omega'$ is obtained by simply differentiating the self-energy $\Sigma(\omega)$ of localized electrons with respect to ε. In the adiabatic approximation in $\Sigma(\omega)$ one must allow only for the contribution from the Coulomb repulsion U. Since the scale on which $\Sigma(\omega)$ varies is much greater than ω_0, we can put $\omega=0$ and employ the Friedel sum rules:

$$\pi n=2\operatorname{Im}\ln G_d(i0^+), \tag{6}$$

where $G_d(i\omega)$ is the analytic continuation of the function

$$G_d(\omega_n)=[i\omega_n-\varepsilon+i\Gamma\operatorname{sign}\omega_n-\Sigma(\omega_n)]^{-1}, \tag{7}$$

and n the average occupation number for the local impurity level. Combining (6) and (7), we get

$$F(0,0)=1+\frac{\partial\Sigma(i0^+)}{\partial\varepsilon}=\frac{2\chi_{ch}}{\pi}\rho_d^{-1}(0), \tag{8}$$

where $\chi_{\text{ch}}=-(1/4)(dn/d\varepsilon)$, and $\rho_d(0)$ is the density of impurity states per impurity on the Fermi level. Allowing for the fact that $|G_d(0)|^2\Gamma/\pi=\rho_d(0)$ and combining Eqs. (8), (4), and (5), we find that

$$\Gamma_i(0,0)=\frac{c}{N^2(0)}[(\chi_{sp}-\chi_{ch})+4\alpha^2\chi_{ch}^2D(0)]. \tag{9}$$

In solving Eq. (2) we use the factorized form of $\Gamma_i(\omega,\omega')$, namely

$$\Gamma_i(\omega,\omega')=\begin{cases}\Gamma(0,0), & 0<\omega,\ \omega'<\overline{\omega},\\ \dfrac{c}{N^2(0)}(\chi_{sp}-\chi_{ch}), & \overline{\omega}<\omega\ \text{(or}\ \ \omega')<\Gamma,\end{cases}$$

where $\overline{\omega}$ is the frequency characterizing the anharmonic oscillator. This is defined below.

The average of the product of Green functions over the positions of impurities, which enters into Eq. (2), is calculated by the usual method[10,11] with a small parameter, the ratio of the electron wavelength to the mean free path. In our case the result of averaging differs from the one obtained in Ref. 11 only by the replacement of function $G_d^0(\omega)$ by the exact value $G_d(\omega)$, with

$$\sum_{\mathbf{k},\mathbf{k}'}[G_{\mathbf{k},\mathbf{k}'}(\omega)G_{-\mathbf{k},-\mathbf{k}'}(-\omega)]_{av}$$

$$\equiv B(\omega)=\frac{\pi N(0)}{|\omega+\pi\Gamma\mathcal{N}|G_d(0)|^2[\omega-\operatorname{Im}\Sigma'(\omega)]|}, \tag{10}$$

where $\mathcal{N}=(c/\pi)N(0)\Gamma$, and $\Sigma'(\omega)=\Sigma(\omega)=\Sigma_{\text{ph}}(\omega)$, in constrast to $\Sigma(\omega)$, incorporates the contribution from lattice vibrations. If $T_c \ll \overline{\omega}$, in substituting (10) into Eq. (2) we can assume, with logarithmic accuracy, that

$$\operatorname{Im}\Sigma'(\omega)=\frac{d\operatorname{Im}\Sigma'(0)}{d\omega}\omega$$

when $\omega<\overline{\omega}$, and, since $\Sigma_{\text{ph}}(\omega)$ rapidly tends to zero when $\omega>\bar{\omega}$,

$$\operatorname{Im}\Sigma'(\omega)=\frac{d\operatorname{Im}\Sigma(0)}{d\omega}\omega$$

for $\overline{\omega}<\omega<\Gamma$. According to Eq. (A6) (see the Appendix),

$$\operatorname{Im}\frac{\partial\Sigma(0)}{\partial\omega}=1-\rho_d^{-1}(0)(\chi_{sp}+\chi_{ch}). \tag{11}$$

In the adiabatic approximation,

$$\operatorname{Im}\frac{\partial\Sigma_{ph}(0)}{\partial\omega}=4\rho_d^{-1}(0)\alpha^2\chi_{ch}^2D(0). \tag{12}$$

Thus,

$$B(\omega)=\frac{\pi N(0)}{|\omega|}\frac{1}{1+\mathcal{N}[\chi_{sp}+\chi_{ch}+A(\omega)]}, \tag{13}$$

where

$$A(\omega)=\operatorname{Im}\frac{\partial\Sigma_{\text{ph}}(0)}{\partial\omega}\theta(\overline{\omega}-\omega).$$

The denominator in (13) determines the renormalization of the density of states at the Fermi surface owing to the resonance scattering of electrons on impurities and to electron-phonon interaction. Combining Eq. (2) with (9) and (13) and the interaction cutoff conditions, we find that

$$T_c=(2\gamma/\pi)\omega_D\exp(-1/\lambda), \tag{14}$$

with γ the Euler constant, ω_D the Debye frequency,

$$\lambda=\frac{\lambda_0+\mathcal{N}(\chi_{ch}-\chi_{sp})a+4\mathcal{N}\chi_{ch}^2\alpha^2D(0)}{1+\lambda_0+\mathcal{N}(\chi_{ch}+\chi_{sp})+4\mathcal{N}\chi_{ch}^2\alpha^2D(0)}$$

$$a=1+\frac{\mathcal{N}(\chi_{sp}-\chi_{ch})\ln(\Gamma/\overline{\omega})}{1+\mathcal{N}(\chi_{ch}+\chi_{sp})}. \tag{15}$$

Here λ_0 is the BCS constant related to the electron-phonon interaction without allowing for impurities, ω_D is assumed to be of the same order of magnitude as $\overline{\omega}$, and the respective contribution of this interaction to $B(\omega)$ is taken into account.

In the absence of interaction of localized electrons with lattice vibrations at $\alpha=0$, Eqs. (15) coincide with the result obtained in Ref. 12 and describe suppression of superconductivity by Anderson impurities.

3. LATTICE DYNAMICS

Equation (15) was derived earlier by one of the authors.[6] Function $D(\omega)$ was calculated in the harmonic approximation. Let us dwell on this aspect. For a harmonic oscillator interacting with an electron by (1) we have

$$\alpha^2D(\omega)=-\frac{\xi\omega_0^2\Gamma}{\omega^2+\omega_0^2[1-\xi\Gamma\Pi(\omega)]}. \tag{16}$$

Allowance for the interaction of localized electrons with lattice vibrations in the adiabatic approximation results only in small corrections to the polarization operator $\Pi(\omega)$. More than that, in the region where $\omega\ll\Gamma$ one can expand $\Pi(\omega)$ in a power series near $\omega=0$. The principal term, $\Pi(0)$, can be expressed in terms of the charge susceptibility as follows:

$$\Pi(0)=-\partial n/\partial\varepsilon=4\chi_{ch}. \tag{17}$$

The value of χ_{ch} as a function of the local-state energy ε reaches its maximum χ_{ch}^* at a certain point ε^*. Combining (16) and (17), we find that at $\xi=\xi_c$, where

$$\xi_c=(4\Gamma\chi_{ch}^*)^{-1}, \tag{18}$$

the natural frequency of the oscillator vanishes and $D(0)\to\infty$. This does not mean, of course, the emergence of a soft mode as in second-order phase transitions. In the case considered here there is no long-range order and "softening" refers only to a single vibrational degree of freedom. Hence, in the region where $|\xi-\xi_c|\ll1$ the quantum fluctuations are great or, in other words, the oscillator's motion is highly anharmonic. To calculate the adiabatic potential energy $U(q)$ of the oscillator, we employ the following formula:

$$\frac{dW}{dq}=\left\langle\frac{\partial(H-T)}{\partial q}\right\rangle=M\omega_0^2q+\alpha n, \tag{19}$$

where T is the oscillator's kinetic energy, and $\langle\cdots\rangle$ denotes averaging over the ground state of the system. At the equilibrium point $q=q_0$, where $dW/dq=0$, we have $M\omega_0^2q_0=-\alpha n_0$. Expanding n, the average occupation number for the level, on the right-hand side of Eq. (19) in powers of $q-q_0$, we find that

$$\frac{dW}{dq}=M\omega_0^2(q-q_0)+\alpha^2\left(\frac{\partial n}{\partial\varepsilon}\right)_{q=q_0}(q-q_0)$$
$$+\sum_{s\geqslant2}\frac{\alpha^{s+1}}{s!}\left(\frac{\partial^sn}{\partial\varepsilon^s}\right)_{q=q_0}(q-q_0)^s. \tag{20}$$

Here we are interested in the critical point $\varepsilon=\varepsilon^*$, at which $\partial^2n/\partial\varepsilon^2=-4\partial\chi_{\text{ch}}/\partial\varepsilon=0$. At $\xi=\xi_c$, the term in (20) linear in $q-q_0$ vanishes. A simple estimate based on dimensional analysis shows that, since $(\omega_0/\Gamma)^{1/3}\ll1$, the terms of orders higher than the third can be discarded in the power series in $q-q_0$. Thus, for $|\xi-\xi_c|\ll1$ and at $\varepsilon=\varepsilon^*$ we have

$$W=\frac{M\omega_0^2}{2}\Delta(q-q_0)^2+b(q-q_0)^4, \tag{21}$$

where

$$\Delta=\left(1-\frac{\xi}{\xi_c}\right),\qquad b=\frac{\alpha^4}{4!}\left(\frac{\partial^3 n}{\partial\varepsilon^3}\right)_{\varepsilon=\varepsilon^*}.$$

As Eq. (21) shows, in the region where $\Delta<0$ the potential energy of the oscillator has two minima. If we set $dW/dq=0$ in Eq. (19), we find how the equilibrium position of the vibrational coordinate is linked to the valence of the impurity. Thus, two different valences of the impurity correspond to two different positions of equilibrium. Note that the emerging instability of the valence and vibrational states occurs even if $U\to\infty$, with only the value of ξ_c changing. At $U=0$ we have $\xi_c=\pi/2$, while at $U=\infty$, as follows from the exact solution of the Anderson model (see Ref. 8), $\xi_c=5.4$. In addition, the term $\chi_{\rm sp}-\chi_{\rm ch}$ in (15), which determines the effect of suppression of superconductivity owing to Coulomb repulsion, is finite for all values of U. This ensures the possibility of T_c rising when the interaction of localized electrons with the lattice vibrations is taken into account.

Knowing the matrix elements of operator q and the energy eigenvalues for an oscillator whose potential energy is defined by (21), we can easily find $D(\omega)$:

$$D(\omega)=-2\sum_m\frac{|q_{0m}|^2\omega_{m0}}{\omega^2+\omega_{m0}^2},\tag{22}$$

where ω_{m0} is the frequency of the transition between the ground and mth excited levels, and we have allowed for the fact that $T_c\ll\omega_{m0}$. The function $D(0)$ was found numerically. The energy eigenvalues of the oscillator were taken from Ref. 13, and the matrix elements were calculated by employing sum rules.[14] In the range of parameters considered here where $|\xi-\xi_c|\ll 1$, the matrix elements q_{0m} with $m>1$ are small compared to q_{01}. Hence, $\overline{\omega}=\omega_{10}$ with a good accuracy. This frequency does not differ too much from ω_0. At $\Delta=0$ we have $\overline{\omega}=0.86(\omega/\Gamma)^{1/3}$. The susceptibilities $\chi_{\rm ch}$ and $\chi_{\rm sp}$ were calculated numerically using the formulas of Ref. 9. Figure 1 depicts the curves representing the dependence of λ on $N=\mathcal{N}/\pi\Gamma$ for three different values of Δ. Obviously, even at $U=\infty$ the transition temperature increases for fairly high concentrations. Note that for a typical value of $N(0)$ of 0.2 state per electron volt per atom and $\Gamma=0.2$ eV, the value $N=1$ is attained at $c\approx 0.1$ per atom. The increase in T_c is more evident in the region where $\Delta<0$. This agrees with the results of calculations by the Monte Carlo method.[7]

The constant λ was calculated by $\varepsilon=\varepsilon^*$. However, for large values of U in the region where $\varepsilon>\varepsilon^*$ the increase in T_c is apparently greater, since $\chi_{\rm sp}$ decreases, as ε grows, faster than $\chi_{\rm ch}$ does, with the result that Coulomb repulsion weakens. The method we used to analyze numerically the Schrödinger equation for an anharmonic oscillator does not enable studying the region $\varepsilon>\varepsilon^*$, where cubic anharmonicity is present in $W(q)$.

4. CONCLUSION

As shown above, Anderson impurities in metals may bring about a considerable increase in T_c if the coupling of the electrons localized on the impurities with lattice vibrations is sufficiently strong and the coupling constant is close to a critical value or even exceeds it. What is important is that for $\xi_c\sim 1$ the electron-phonon interaction is not necessarily strong in the sense of the dependence of electron energies (constant α in our case) or other energy parameters of electrons on the displacements of lattice atoms. As noted in Ref. 7, such values of ξ correspond to an ordinary or even weak electron-phonon interaction in metals.

The presence of a strong Coulomb repulsion of the electron on an inpurity has no marked effect on T_c, at least in the region where $|\xi-\xi_c|\ll 1$. Although the increase in T_c is much stronger at $U=0$, it is also quite noticeable at $U=\infty$.

It is still difficult to say to what extent this mechanism of the increase in T_c can be employed to explain the high values of T_c in superconducting cupric oxides. There is massive indirect evidence in favor of this mechanism (see, e.g., Ref. 15). Also of interest is the empirical relation between T_c for a broad class of high-temperature superconductors and the energy of an electron localized on oxygen atoms at the vertices of the pyramids surrounding the copper atoms.[16] For the same atoms in $\rm YBa_2Cu_3O_7$, the x-ray absorption spectra near the threshold exhibit the presence of two positions of equilibrium along the c axis that are degenerate or differ slightly in energy.[17] The main problem in the attempts to apply this model to high-T_c superconducting oxides remains its extension to the region of high impurity concentrations, with, say, special kinds of defects[15] (oxygen vacancies) acting as impurities or with impurities at the sites of a dense regular lattice.

APPENDIX

Let us obtain the differential formulas for Matsubara's Green functions in the same way as is done in the theory of a Fermi liquid.[10] We place the system in a slowly varying homogeneous field that acts only on spins pointing upward (↑). Allowing for the fact that the total number of particles with a given projection of spin on the z axis is conserved, we

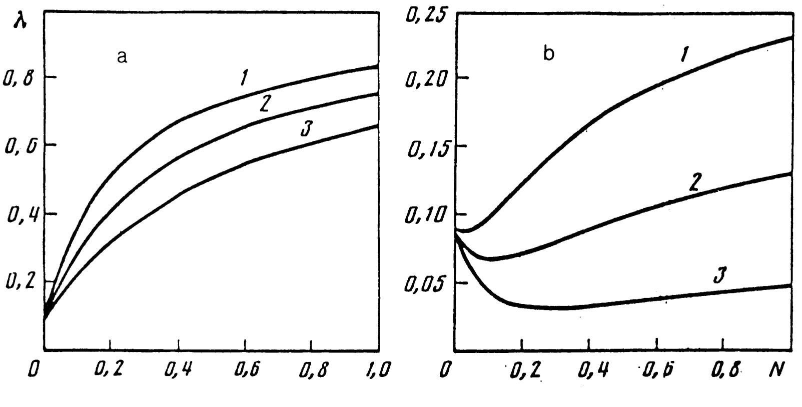

FIG. 1. The dependence of λ on the impurity concentration N for $\omega_0/\Gamma=0.1$ and $\lambda_0=0.1$ with (a) $U=0$ and (b) $U=\infty$. Curves *1* correspond to $\Delta=-0.1$, curves *2* to $\Delta=0$, and curves *3* to $\Delta=0.1$.

see that finding the variation in $G_{d\uparrow}(\omega)$ amounted to differentiating $G_{d\uparrow}(\omega)$ with respect to frequency, while the variation in $G_{d\downarrow}$ is nil. On the other hand, these variations can be found in the first approximation in the external field. As a reult we arrive at the following formulas:

$$\frac{\partial G_d(\omega)}{\partial i\omega}=-G_d^2(\omega)\left\{1+\int\Gamma_{\uparrow\uparrow}(\omega,\omega')\right.$$

$$\left.\times[G^2(\omega')+2\pi\rho_d(0)\delta(\omega')]\frac{d\omega'}{2\pi}\right\}$$

$$-\rho_d(0)\delta(\omega), \tag{A1}$$

$$0=\int\Gamma_{\uparrow\downarrow}(\omega,\omega')[G^2(\omega')+2\pi\rho_d(0)\delta(\omega')]\frac{d\omega'}{2\pi}. \tag{A2}$$

Here $\Gamma_{\sigma\sigma'}(\omega,\omega')$ is the total vertex of two-particle interaction with two lines in, (ω,σ) and (ω',σ'), and two similar lines out. The temperature is assumed low, so that summation over discrete frequencies is replaced with integration. The terms proportional to $\delta(\omega)$ on the right-hand sides of Eqs. (A1) and (A2) are related to the contribution from the conduction electron as follows:

$$\lim_{\nu\to 0}\sum_{\mathbf{k}}[G_{d\mathbf{k}}(\omega)G_{\mathbf{k}d}(\omega+\nu)]$$

$$=|V|^2\lim_{\nu\to 0}\left[G_d(\omega)G_d(\omega+\nu)\sum_{\mathbf{k}}\frac{1}{i\omega-\varepsilon_{\mathbf{k}}}\frac{1}{i(\omega+\nu)-\varepsilon_{\mathbf{k}}}\right]$$

$$=2\pi N(0)|V|^2|G_d(0)|^2\delta(\omega)=2\pi\rho_d(0)\delta(\omega).$$

Now we determine the susceptibility:

$$\rho_d(0)\chi_{\sigma\sigma'}=\operatorname{sign}\sigma\operatorname{sign}\sigma'\int_0^\beta d\tau\langle[n_\sigma(\tau)-\langle n_\sigma\rangle][n_{\sigma'}(0)-\langle n_{\sigma'}\rangle]\rangle. \tag{A3}$$

This implies that

$$\rho_d(0)\chi_{\sigma\sigma'}=-\delta_{\sigma\sigma'}\int G^2(\omega)\frac{d\omega}{2\pi}$$

$$-\operatorname{sign}\sigma\operatorname{sign}\sigma'\int G^2(\omega)\Gamma_{\sigma\sigma'}(\omega,\omega')G^2(\omega')\frac{d\omega}{2\pi}\frac{d\omega'}{2\pi}. \tag{A4}$$

Multiplying Eq. (A2) by $\widetilde{G}^2(\omega)$, integrating the product with respect to ω, and employing (A4), we find that

$$\chi_{\uparrow\downarrow}=\rho_d(0)\Gamma_{\uparrow\downarrow}(0,0), \tag{A5}$$

where we have used (A2) at point $\omega=0$. One more equation can be obtained by integrating Eq. (A1) with respect to ω. Substituting the result into Eq. (A4) with $\sigma=\sigma'$ and using the obvious equality $\Gamma_{\sigma\sigma}(0,0)=0$ and the Dyson equation for $G_d(\omega)$, we find that

$$\left.\frac{\partial\Sigma}{\partial i\omega}\right|_0=1-\chi_{\uparrow\uparrow}. \tag{A6}$$

The susceptibilities $\chi_{\uparrow\downarrow}$ and $\chi_{\uparrow\uparrow}$ are in turn expressed in terms of χ_{ch} and χ_{sp}. Equations (A5) and (A6) coincide with those obtained in Ref. 18 for the symmetric Anderson model, where the symmetries have been used explicitly. As we see, there is no need for this.

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Translated by Eugene Yankovsky