

## Theory for dirty superconductors. II. McMillan solution and $T_c$ degradation

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For a recent strong-coupling theory for dirty superconductors, a solution for  $T_c$  of the McMillan type is obtained, which still contains complete disorder renormalizations of both anomalous and normal self-energies. All disorder effects leading to diffusion enhancement of vertices are calculated. The resulting  $T_c$  formula gives good account of the observed  $T_c$  degradation in high- $T_c$  materials. A detailed discussion of the approximations used and of the relation to previous approaches is given.

### I. INTRODUCTION

Understanding the properties of disordered superconductors has proven to be a difficult task. Even before a theoretical understanding of clean superconductivity<sup>1</sup> was obtained, experiments indicated that many weak-coupling superconductors show an enhancement of  $T_c$  if they are made disordered.<sup>2,3</sup> On the contrary, low- $T_c$  strong-coupling materials like Hg and Pb show a small decrease of  $T_c$  with increasing disorder.<sup>3</sup> For most materials, these are very small effects (at most 20%) compared to the strong destructive effects of magnetic impurities. In recent years, interest in the disorder dependence of  $T_c$  has been revived as more and more high- $T_c$  ( $T_c \geq 10$  K) superconducting materials have been found. Most members of this class are fairly strongly disordered from the point of view of metal physics, with resistivities  $\rho \geq 20 \mu\Omega \text{ cm}$ . Invariably, the cleanest specimens are those with the highest  $T_c$ , and  $T_c$  decreases rapidly with increasing disorder.<sup>4,5</sup> Thereby the slope  $dT_c/d\rho$  is steeper the higher the  $T_c$  in the clean limit. In contrast to the disorder dependence of  $T_c$  in low- $T_c$  materials, this  $T_c$  degradation is by no means a small effect.<sup>6</sup> For instance, in Nb<sub>3</sub>Ge,  $T_c$  drops from 22 to 5 K if  $\rho$  is increased from 40 to 120  $\mu\Omega \text{ cm}$  by means of irradiation.<sup>4</sup>

There has been a number of theoretical efforts to understand these various phenomena.<sup>7-11</sup> These have been discussed in a preceding paper,<sup>12</sup> and we will not repeat this discussion here. In the same paper,<sup>12</sup> a new strong-coupling theory for dirty superconductors was developed. This was shown to yield a unified description of all the effects discussed in Refs. 7-11, and to contain additional disorder renormalizations of the same order of magnitude, which had not been considered so far. It turned out that from a microscopic point of view, the effects discussed in Refs. 10 and 11 are due to impurity renormalization of that part of the normal self-energy which is an even function of frequency and can be neglected in standard theory. This led to the introduction of a new renormalization function  $Y$  in addition to the anomalous self-energy  $W$  and the usual renormalization function  $Z$ . The resulting strong-coupling equations are coupled integral equations for three self-energies  $W$ ,  $Y$ , and  $Z$ , which depend on energy as well as frequency. These equations are rather

complicated and have not been solved so far. However, a detailed discussion has been given in Ref. 12 of how the previous strong-coupling approaches are obtained as special cases of the new theory. Comparison with Ref. 10 was more difficult because of the different models. Apart from that, a new mechanism for an enhancement of  $\lambda$  has been identified. This was found to be of an importance equal to the effects discussed previously (apart from Ref. 7, they are all due to diffusion enhanced vertices). Since there are so many effects of comparable magnitude, it is clear that for the previous approaches, each of which had taken into account one of them, a meaningful comparison with experiment is not possible. Rather one must demand as a minimum requirement for such a comparison that all impurity renormalizations belonging to some most important class be taken into account (if such a classification is possible).

The purpose of the present paper is to present a calculation of  $T_c$  which meets the above minimum requirement within the framework provided in Ref. 12 (hereafter referred to as I). To this end we first obtain an approximate solution at  $T_c$  of the integral equations given in I, without specifying the various disorder renormalizations. This will be done by approximating the energy dependence of the new renormalization function  $Y$  in such a way that the integral with respect to the energy can be carried out. The resulting two integral equations have the same structure as the standard strong-coupling theory.<sup>13</sup> Therefore we can use McMillan's method<sup>14</sup> to obtain an approximate solution. Then the impurity renormalizations of the vertices are calculated in lowest order of the systematic procedure given in I. This way we keep only the most dominant disorder contributions, that is, diffusion enhancement of vertices. We will find this sufficient to describe the relatively strong effects on  $T_c$  found in the high- $T_c$  strong-coupling materials. The resulting generalized McMillan formula contains the  $T_c$  formula obtained before,<sup>10</sup> but now both  $\lambda$  and  $\mu$  are disorder dependent. So this result confirms and extends that of Ref. 10. We compare with a number of experiments on high- $T_c$  materials, and find good agreement for resistivities which are not too large. For  $\rho \geq 100-200 \mu\Omega \text{ cm}$ , depending on the material, the experiments find  $T_c$  to decrease faster than described by the theory. The probable reasons for

this discrepancy are discussed in a continuation of the discussion given in I.

## II. APPROXIMATE SOLUTION FOR THE STRONG-COUPLING EQUATIONS

### A. Integral equations

The general integral equations determining the self-energies and Green's functions have been given in Eqs.

$$W(\omega) = \int d\nu \alpha^2 F^F(\nu) \int \frac{dx}{\pi} \int d\epsilon' \text{Im}F(\epsilon', x) \left[ \frac{f(x)}{x-\omega-\nu} + \frac{1-f(x)}{x-\omega+\nu} \right] + U_c^W \int \frac{dx}{\pi} f(x) \int d\epsilon' \text{Im}F(\epsilon', x), \quad (2.1)$$

$$\omega[1-Z(\omega)] = \int d\nu \alpha^2 F^F(\nu) \int \frac{dx}{\pi} \int d\epsilon' \text{Im}G(\epsilon', x) \omega \left[ \frac{f(x)}{(x-\nu)^2-\omega^2} + \frac{1-f(x)}{(x+\nu)^2-\omega^2} \right], \quad (2.2)$$

$$Y(\epsilon, \omega) = \int d\nu \int d\epsilon' \alpha^2 F^F(\epsilon-\epsilon', \nu) \int \frac{dx}{\pi} \text{Im}G(\epsilon', x) \left[ f(x) \frac{x-\nu}{(x-\nu)^2-\omega^2} + [1-f(x)] \frac{x+\nu}{(x+\nu)^2-\omega^2} \right] + \int d\nu \int d\epsilon' \left[ \frac{4}{\nu} \alpha^2 F^H(\epsilon-\epsilon', \nu) + U_c^Y(\epsilon-\epsilon')\delta(\nu) \right] \int \frac{dx}{\pi} f(x) \text{Im}G(\epsilon', x). \quad (2.3)$$

The retarded Green's functions read

$$G(\epsilon, \omega) = \frac{\omega Z(\omega) + [\epsilon + Y(\epsilon, \omega)]}{[\omega Z(\omega)]^2 - [\epsilon + Y(\epsilon, \omega)]^2 - W(\omega)^2}, \quad (2.4a)$$

$$F(\epsilon, \omega) = \frac{-W(\omega)}{[\omega Z(\omega)]^2 - [\epsilon + Y(\epsilon, \omega)]^2 - W(\omega)^2}. \quad (2.4b)$$

$f(x)$  denotes the Fermi function, and the disorder-dependent Eliashberg functions are defined as

$$\alpha^2 F^{F,H}(\epsilon, \nu) = \sum_{q,b} R_b^{F,H}(\mathbf{q}, \epsilon) B_b(\mathbf{q}, \nu), \quad (2.5)$$

with  $\alpha^2 F^F(\nu) \equiv \alpha^2 F^F(\epsilon=0, \nu)$ .  $B_b$  is the phonon spectral function for polarization branch  $b$ , and the vertex functions  $R_b^{F,H}$  have been defined in I, Eqs. (3.7') and (3.10), in terms of electronic correlation functions. Finally, the Coulomb kernels are given by

$$U_c^W = \sum_{q \neq 0} R_c^F(\mathbf{q}, 0) \frac{\kappa^2/2N_F}{q^2 + \kappa^2}, \quad (2.6a)$$

$$U_c^Y(\epsilon) = \sum_{q \neq 0} [R_c^F(\mathbf{q}, \epsilon) - 2R_c^H(\mathbf{q}, \epsilon)] \frac{\kappa^2/2N_F}{q^2 + \kappa^2}. \quad (2.6b)$$

Here  $\kappa$  is the Thomas-Fermi screening wave number and  $N_F$  is the density of states per spin at the Fermi level. For the definition of  $R_c^{F,H}$  in terms of correlation functions we refer again to I, Eqs. (3.14) and (3.15).

### B. Energy integration

The main obstacle to solving Eqs. (2.1)–(2.3) with the methods known from standard strong-coupling theory is the energy dependence of  $Y$ . To deal with this difficulty, we first remember that in the clean limit,  $Y$  can be neglected.<sup>15</sup> We note that in the following we will calculate correlation functions within a jellium model, neglect-

(4.12)–(4.14) of I. Instead of writing them down again in full, we immediately make a number of simplifications. It has already been discussed in I that the energy dependence of the anomalous self-energy  $W$  and the renormalization function  $Z$  can be neglected within the range of validity of the theory. We also neglect thermal phonons.<sup>14</sup> Then we have the following equations for the retarded self-energies:

ing band-structure effects. Therefore, by “clean limit” we mean here and in the following, “clean limit of a jellium model” (cf. Ref. 12 of I). So we have to consider only  $\delta Y = Y - Y^{(0)}$ , where  $Y^{(0)}$  is the contribution for zero disorder. Now we expand  $\delta Y$  in a Taylor series with respect to  $\epsilon$ , and terminate at the linear term:

$$\delta Y(\epsilon, \omega) = \delta Y(0, \omega) + \epsilon Y'(\omega). \quad (2.7)$$

We anticipate that  $Y(0, \omega)$  is zero within our approximation scheme, and that  $Y'$  is independent of  $\omega$  (we will verify this later). Then the Green's functions, Eqs. (2.4), can be written as

$$G(\epsilon, \omega) = \frac{1}{1+Y'} \frac{\omega \bar{Z}(\omega) + \epsilon}{[\omega \bar{Z}(\omega)]^2 - \epsilon^2 - \bar{W}(\omega)^2}, \quad (2.8a)$$

$$F(\epsilon, \omega) = \frac{1}{1+Y'} \frac{-\bar{W}(\omega)}{[\omega \bar{Z}(\omega)]^2 - \epsilon^2 - \bar{W}(\omega)^2}. \quad (2.8b)$$

Here we have introduced  $\bar{Z}(\omega) = Z(\omega)/(1+Y')$  and  $\bar{W}(\omega) = W(\omega)/(1+Y')$ . The  $\epsilon$  dependence of  $G$  and  $F$  is now elementary, and we can perform the energy integrations in Eqs. (2.1) and (2.2). We define  $-i\pi\mathcal{G}(\omega) = \int d\epsilon G(\epsilon, \omega)$  and  $i\pi\mathcal{A}(\omega) = \int d\epsilon F(\epsilon, \omega)$ , and obtain

$$\mathcal{G}(\omega) = \frac{1}{1+Y'} \frac{\omega \bar{Z}(\omega) \text{sgn}(\omega)}{[\omega^2 \bar{Z}(\omega)^2 - \bar{W}(\omega)^2]^{1/2}}, \quad (2.9a)$$

$$\mathcal{A}(\omega) = \frac{1}{1+Y'} \frac{\bar{W}(\omega) \text{sgn}(\omega)}{[\omega^2 \bar{Z}(\omega)^2 - \bar{W}(\omega)^2]^{1/2}}. \quad (2.9b)$$

Notice that  $\text{Re}\mathcal{G}(\omega)$  is an even function of frequency. Inspection of the first term in Eq. (2.3) shows that indeed  $Y(0, \omega) = 0$ ,<sup>16</sup> so the first assumption made after Eq. (2.7) was consistent. We can now write Eqs. (2.1) and (2.2) as follows:

$$W(\omega) = -U_c^W \int_0^\infty dx \tanh(x/2T) \operatorname{Re} \mathcal{A}(x) + \int d\nu \alpha^2 F^F(\nu) \int dx \operatorname{Re} \mathcal{A}(x) \left[ \frac{f(x)}{x-\omega-\nu} + \frac{1-f(x)}{x-\omega+\nu} \right], \quad (2.10)$$

$$\omega[1-Z(\omega)] = - \int d\nu \alpha^2 F^F(\nu) \int dx \operatorname{Re} \mathcal{A}(x) \left[ \frac{f(x)}{x-\omega-\nu} + \frac{1-f(x)}{x-\omega+\nu} \right]. \quad (2.11)$$

We still have to determine  $Y'$ . From Eq. (2.3), we obtain

$$\begin{aligned} \delta Y(\epsilon, \omega) = \int d\epsilon' \int d\nu \left[ \delta \alpha^2 F^F(\epsilon - \epsilon', \nu) \int \frac{dx}{\pi} \operatorname{Im} G(\epsilon', x) \left[ f(x) \frac{x-\nu}{(x-\nu)^2 - \omega^2} + [1-f(x)] \frac{x+\nu}{(x+\nu)^2 - \omega^2} \right] \right. \\ \left. + \left[ \frac{4}{\nu} \alpha^2 F^H(\epsilon - \epsilon', \nu) + \delta U_c^Y(\epsilon - \epsilon') \delta(\nu) \right] \int \frac{dx}{\pi} f(x) \operatorname{Im} G(\epsilon', x) \right]. \quad (2.12) \end{aligned}$$

$\delta \alpha^2 F^F$  and  $\delta U_c^Y$  denote the quantities given by Eqs. (2.5) and (2.6b), with the respective clean-limit contributions subtracted.  $\alpha^2 F^H$  is a Hartree contribution, which vanishes in the clean limit. According to Eq. (2.7), we have  $Y'(\omega) = d\delta Y(\epsilon, \omega)/d\epsilon|_{\epsilon=0}$ . Under the integral, we may differentiate with respect to  $\epsilon'$  instead of  $\epsilon$ , and integration by parts yields

$$\begin{aligned} Y'(\omega) = \int d\nu \int \frac{dx}{\pi} \left[ \delta \alpha^2 F^F(\nu) \left[ f(x) \frac{x-\nu}{(x-\nu)^2 - \omega^2} + [1-f(x)] \frac{x+\nu}{(x+\nu)^2 - \omega^2} \right] \right. \\ \left. + \left[ \frac{4}{\nu} \alpha^2 F^H(\nu) + \delta U_c^Y \delta(\nu) \right] f(x) \right] \lim_{\epsilon \rightarrow \infty} [\operatorname{Im} G(\epsilon, x) - \operatorname{Im} G(-\epsilon, x)]. \quad (2.13) \end{aligned}$$

From Eq. (2.8a), we see that for  $|\epsilon| \rightarrow \infty$ ,  $\operatorname{Im} G(\epsilon, x)$  is nonzero only if  $|x| \rightarrow \infty$  as well. Consequently, the  $\omega$ -dependent part of  $Y'$  vanishes as we have anticipated after Eq. (2.7), and

$$Y' = \int d\nu \left[ \frac{4}{\nu} \alpha^2 F^H(\nu) + \delta U_c^Y \delta(\nu) \right] \int \frac{dx}{\pi} f(x) \lim_{\epsilon \rightarrow \infty} [\operatorname{Im} G(\epsilon, x) - \operatorname{Im} G(-\epsilon, x)]. \quad (2.13')$$

Equations (2.9), (2.10), (2.11), and (2.13) form a new set of self-consistency equations, which have been considerably simplified in comparison with the original ones. We will now solve them for  $T_c$ .

### C. McMillan solution for $T_c$

As usual, we define the gap parameter  $\Delta(\omega) = W(\omega)/Z(\omega) = \overline{W}(\omega)/\overline{Z}(\omega)$ . For  $T \rightarrow T_c$ , we have  $W \rightarrow 0$ , so we can substitute  $\operatorname{Re} \mathcal{A}(\omega) = 1/(1+Y')$ ,  $\operatorname{Re} \mathcal{A}(\omega) = [1/(1+Y')] \operatorname{Re} \Delta(\omega)/\omega$  into the right-hand side of Eqs. (2.10) and (2.11). This yields

$$\omega[1-Z(\omega)] = \frac{1}{1+Y'} \int d\nu \alpha^2 F^F(\nu) \int_0^\infty dx \left[ f(-x) \left[ \frac{1}{x+\nu+\omega} - \frac{1}{x+\nu-\omega} \right] + f(x) \left[ \frac{1}{-x+\nu+\omega} - \frac{1}{-x+\nu-\omega} \right] \right], \quad (2.14)$$

$$\begin{aligned} \Delta(\omega)Z(\omega) = \frac{-U_c^W}{1+Y'} \int_0^\infty \frac{dx}{x} \tanh(x/2T) \operatorname{Re} \Delta(x) \\ + \frac{1}{1+Y'} \int d\nu \alpha^2 F^F(\nu) \int_0^\infty \frac{dx}{x} \operatorname{Re} \Delta(x) \left[ f(-x) \left[ \frac{1}{x+\nu+\omega} + \frac{1}{x+\nu-\omega} \right] \right. \\ \left. - f(x) \left[ \frac{1}{-x+\nu+\omega} + \frac{1}{-x+\nu-\omega} \right] \right]. \quad (2.15) \end{aligned}$$

To calculate  $Y'$  from Eq. (2.13'), we need to know  $\operatorname{Im} G$  at  $T_c$ . At  $T_c$ , we have  $\Delta(\omega) = 0$ , but  $Z(\omega) \neq 1$ . So

$$\int \frac{dx}{\pi} f(x) \operatorname{Im} G(\epsilon, x) = - \int dx f(x) \delta[xZ(x) - \epsilon(1+Y')],$$

and we have to change variables  $x \rightarrow x' = xZ(x)$ . From Eq. (2.14), we see that  $Z(x \rightarrow \infty) = 1 + O(1/x^2)$ ; hence,  $\lim_{x \rightarrow \infty} x dZ/dx = 0$ , and therefore  $\lim_{x \rightarrow \infty} [Z(x) + x dZ/dx] = Z(\infty) = 1$ . Consequently, at those large frequencies we are interested in, the Jacobian is one, and we find

$$\int \frac{dx}{\pi} f(x) \lim_{\epsilon \rightarrow \infty} [\text{Im}G(\epsilon, x) - \text{Im}G(-\epsilon, x)] \\ = f(-\infty) - f(\infty) \\ = 1.$$

This yields for  $Y'$  the simple result

$$Y' = \delta U_c^Y + 4 \int \frac{dv}{v} \alpha^2 F^H(v). \quad (2.16)$$

Inspection of Eqs. (2.14) and (2.15) shows that, apart from the factor  $1/(1+Y')$ , they have the same structure as in the clean case. Therefore we can immediately write down our generalization of McMillan's<sup>14</sup> result for  $T_c$ :<sup>17</sup>

$$T_c = \frac{\Theta_D}{1.45} \exp \left[ - \frac{1.04(1 + \tilde{\lambda} + Y')}{\tilde{\lambda} - \mu^* [1 + 0.62\tilde{\lambda}/(1 + Y')]} \right], \quad (2.17a)$$

where

$$\tilde{\lambda} = 2 \int \frac{dv}{v} \alpha^2 F^F(v) \quad (2.17b)$$

and

$$\mu^* = U_c^W \left[ 1 + \frac{U_c^W}{1 + Y'} \ln(E_B / \hbar\omega_0) \right]^{-1}. \quad (2.17c)$$

Here  $E_B$  is of the order of the bandwidth and  $\omega_0$  is of the order of the Debye frequency. Notice that  $\tilde{\lambda}$ ,  $Y'$ , and  $U_c^W$  all depend on disorder. What remains to be done is to calculate this disorder dependence.

$$U_c^W = \mu + \frac{\kappa^2/2N_F}{\pi N_F} \sum_q \frac{g(q)}{Dq^2} \left[ \frac{1 - \delta_{q,0}}{q^2 + \kappa^2} + \frac{1}{g^2(q)} \sum_{\mathbf{k}, \mathbf{p}} \sum_{\mathbf{k}', \mathbf{p}'} g_{\mathbf{k}\mathbf{k}'}(\mathbf{q}) \frac{1 - \delta_{\mathbf{k}, \mathbf{p}}}{(\mathbf{k} + \mathbf{p})^2 + \kappa^2} g_{\mathbf{p}'\mathbf{p}}(\mathbf{q}) \right], \quad (2.20)$$

with diffusion constant  $D$  and the static phase-space correlation function

$$g_{\mathbf{k}\mathbf{p}}(\mathbf{q}) = [c_{\mathbf{k}-\mathbf{q}/2}^\dagger c_{\mathbf{k}+\mathbf{q}/2} | c_{\mathbf{p}-\mathbf{q}/2}^\dagger c_{\mathbf{p}+\mathbf{q}/2} ]. \quad (2.21)$$

The  $c^\dagger, c$  are electronic creation and annihilation operators and  $[ | ]$  denotes the Kubo product defined in I.  $g_{\mathbf{k}\mathbf{p}}$  is understood to contain disorder, but no electron-electron or electron-phonon interactions. It can be calculated, e.g., in the self-consistent Born approximation.<sup>19</sup> In consideration of the crude approximations we have made already, however, this does not seem worthwhile. We therefore simply replace  $g_{\mathbf{k}\mathbf{p}}$  by the free-fermion correlation<sup>20</sup>

$$g_{\mathbf{k}\mathbf{p}}^{(0)}(\mathbf{q}) = -\delta_{\mathbf{k}\mathbf{p}}(m/\mathbf{k}\mathbf{q}) \{ \Theta[k_F^2 - (\mathbf{k} + \mathbf{q}/2)^2] \\ - \Theta[k_F^2 - (\mathbf{k} - \mathbf{q}/2)^2] \}. \quad (2.22)$$

In this approximation, the static density correlation  $g^{(0)}(\mathbf{q}) = \sum_{\mathbf{k}, \mathbf{p}} g_{\mathbf{k}\mathbf{p}}^{(0)}(\mathbf{q})$  is just the Lindhard function. It shows the asymptotic behavior  $g^{(0)}(q=0) = N_F$ ,  $g^{(0)}(q \gg 2k_F) = 0(1/q^2)$ , and we replace it by a step function:  $g^{(0)}(q) \simeq N_F \Theta(2k_F - q)$ . Finally, the  $q$  dependence

#### D. Disorder renormalizations and $T_c$ formula

We start with the Coulomb kernels  $U_c^W$  and  $U_c^Y$ . According to Eqs. (2.6) they are determined by the functions  $R_c^F$  and  $R_c^H$ , which in turn have been defined in Eqs. (3.14) and (3.15) of I. To calculate them, we follow the general scheme given in Appendix B of I. Accordingly, we first consider the clean case, denoted by the superscript (0). From Eq. (2.16) we have  $(Y')^{(0)} = 0$ , while  $(U_c^W)^{(0)}$  has already been calculated in I. The result was the effective Coulomb potential given by Morel and Anderson,<sup>18</sup> viz.,

$$(U_c^W)^{(0)} \equiv \mu = \frac{1}{2}(\kappa/2k_F)^2 \ln[1 + (2k_F/\kappa)^2], \quad (2.18)$$

where  $k_F$  is the Fermi wave number. Using the free-fermion correlation function in Eq. (2.5), we find from Eq. (2.17b) the known result,<sup>7</sup>

$$\tilde{\lambda}^{(0)} \equiv \lambda = 2g_L^2 N_F \int \frac{dv}{v} \int_0^{2k_F} dq (q/2k_F^2) B_L^{(0)}(q, v). \quad (2.19)$$

Here  $g_L = k_F^2/3m(\rho_i)c_L^{1/2}$  with ion mass density  $\rho_i$  and longitudinal sound velocity  $c_L$ .  $B_L^{(0)}$  is the longitudinal phonon spectrum in the clean limit.

In lowest order of the general approximation scheme only diffusive disorder contributions are kept. For this case, the renormalization of  $U_c^W$  has already been given in Eq. (5.10) of I. The result was

of the second contribution to  $\delta U_c^W$  in Eq. (2.20) is not important, since the same kind of  $q$  dependence appears in the numerator as well as in the denominator. We therefore ignore it, using  $g_{\mathbf{k}\mathbf{p}}^{(0)}(q=0) = \delta_{\mathbf{k}\mathbf{p}} 2m\delta(k_F^2 - k^2)$ . This way we obtain

$$U_c^W = \mu \left[ 1 + (1 + \xi) \frac{6}{\pi} (\rho/\rho_M) \right]. \quad (2.23)$$

Here the resistivity  $\rho$  has been used as a measure of the disorder. It is connected with the diffusion constant by  $\rho = 1/2N_FD$ . The resistivity scale is given by Mott's resistivity  $\rho_M = 3\pi^2/k_F$ . It is that value of the Drude resistivity which is obtained for a mean free path  $l = 1/k_F$ . The present theory is valid for  $\rho/\rho_M \ll 1$ . The parameter  $\xi$  is given by

$$\xi = (2k_F/\kappa) \arctan(2k_F/\kappa) \ln[1 + (2k_F/\kappa)^2]. \quad (2.24)$$

For the other disorder-dependent quantities, we use exactly the same reasoning. Repeating the arguments which led to Eq. (5.10), of I or Eq. (2.20), we obtain

$$\delta U_c^Y = \frac{\kappa^2/2N_F}{\pi N_F} \sum_q \frac{g(q)}{Dq^2} \left[ \frac{1-\delta_{q,0}}{q^2+\kappa^2} - \frac{3}{g^2(q)} \sum_{\mathbf{k},\mathbf{p}} \sum_{\mathbf{k}',\mathbf{p}'} g_{\mathbf{k}\mathbf{k}'}(\mathbf{q}) \frac{1-\delta_{\mathbf{k},\mathbf{p}}}{(\mathbf{k}-\mathbf{p})^2+\kappa^2} g_{\mathbf{p}\mathbf{p}'}(\mathbf{q}) \right]. \quad (2.25)$$

The same approximations which led to Eq. (2.23), yield

$$\delta U_c^Y = \mu(\zeta-3) \frac{6}{\pi} (\rho/\rho_M). \quad (2.26)$$

The expressions for the phonon kernels  $\delta\alpha^2 F^F$  and  $\alpha^2 F^H$  which correspond to Eqs. (5.10) of I or (2.20) and (2.25) are rather lengthy because of the tensor vertices entering the electron-phonon coupling. Since the analogy to the Coulomb case is perfect, we do not have to write them down. To evaluate the terms

$$\sum_{\mathbf{k},\mathbf{p}} \sum_{\mathbf{k}',\mathbf{p}'} g_{\mathbf{k}\mathbf{k}'}(\mathbf{q}) B_b(\mathbf{k}\pm\mathbf{p},\nu) g_{\mathbf{p}\mathbf{p}'}(\mathbf{q}),$$

occurring in these expressions, we again neglect the  $q$  dependence and use a Debye spectrum  $B_b(\mathbf{q},\nu)$

$= \frac{1}{2} c_b q \delta(\nu - c_b q) \Theta(\omega_D - \nu)$ . Then we obtain

$$2 \int \frac{d\nu}{\nu} \delta\alpha^2 F^F(\nu) = \lambda \frac{6}{\pi} (\rho/\rho_M), \quad (2.27a)$$

$$2 \int \frac{d\nu}{\nu} \delta\alpha^2 F^H(\nu) = 2\lambda \frac{6}{\pi} (\rho/\rho_M). \quad (2.27b)$$

The factor-of-2 difference between Eqs. (2.24a) and (2.24b) stems from the fact that the exchange term has only one diffusive contribution (due to Cooper-propagator renormalization), while the direct one has two of them (cf. the discussion in I).

We now can collect our results. Combining Eqs. (2.16), (2.17), (2.23), and (2.27), we obtain the generalized McMillan formula

$$T_c = \frac{\Theta_D}{1.45} \exp \left[ - \frac{1.04[1 + \lambda f_1(\hat{\rho}) + f_2(\hat{\rho})]}{\lambda f_1(\hat{\rho}) - \mu^*(\hat{\rho}) \{1 + 0.62\lambda f_1(\hat{\rho})/[1 + f_2(\hat{\rho})]\}} \right]. \quad (2.28)$$

Here  $\hat{\rho} = \rho/\rho_M$  is the dimensionless resistivity, the disorder-dependent Coulomb pseudopotential is given by

$$\mu^*(\hat{\rho}) = \mu f_3(\hat{\rho}) \left[ 1 + \frac{\mu f_3(\hat{\rho})}{1 + f_2(\hat{\rho})} \ln(E_B/\hbar\omega_0) \right]^{-1}, \quad (2.29)$$

and the three disorder renormalization functions read

$$f_1(x) = 1 + (6/\pi)x, \quad (2.30a)$$

$$f_2(x) = [\mu(\zeta-3) + 4\lambda](6/\pi)x, \quad (2.30b)$$

$$f_3(x) = 1 + (1+\zeta)(6/\pi)x. \quad (2.30c)$$

$\lambda$  is the clean-limit parameter which can be measured (at least in principle), and is well known for many materials.<sup>21</sup>  $\mu$  and  $\zeta$  are given by the screening parameter  $2k_F/\kappa$ . The latter should not be very sensitive to moderate disorder, and in the clean limit reliable values exist for many substances. The least-well-known parameters remaining are  $\ln(E_B/\hbar\omega_0)$  and the resistivity scale  $\rho_M$ . The former is present in the clean limit as well, and is usually assumed to have a value of 5–6. However, for transition metals it might be considerably smaller.<sup>9</sup>  $\rho_M$  is not directly measurable. Since it sets the scale for the critical regime of the Anderson transition, however, one has an idea about its order of magnitude. For most materials, values of the order of 1000  $\mu\Omega$  cm seem to be consistent with what is known about the Anderson transition. Equations (2.28)–(2.30) represent the leading disorder corrections to McMillan's formula in the sense that the first nontrivial contribution of  $Y$  has been taken into account, and all of the strongest disorder renormalizations; that is, diffusive vertex enhancements, have been included.

### III. RESULTS AND DISCUSSIONS

#### A. Connection with previous calculations

We have already discussed at length, both in I and in the preceding section, our approach in general as well as the particular approximations that led to Eq. (2.28). Here we briefly show how our result is related to previous work, in particular to Ref. 10.

Let us ignore for a while the disorder renormalization of  $\lambda$  by putting  $f_1(x) \equiv 1$ , as well as that of  $\mu[f_3(x) \equiv 1]$ , and assume  $\lambda$  to be small (weak coupling). Then we have

$$T_c \sim \exp \left[ - \frac{1+f_2}{\lambda - \mu \left/ \left[ 1 + \frac{\mu}{1+f_2} \ln(E_B/\hbar\omega_0) \right] \right.} \right].$$

If we additionally assume the disorder to be weak, we can write  $1+f_2 \simeq 1/(1-f_2)$  and obtain

$$T_c \sim \exp \left[ \frac{-1}{(\lambda - \mu^*)(1-f_2)} \right], \quad (3.1a)$$

$$\mu^* = \mu [1 + \mu(1-f_2)\ln(E_B/\hbar\omega_0)]^{-1}. \quad (3.1b)$$

This is the structure of the result obtained previously,<sup>10,22</sup> and inspection of  $f_2$ , Eq. (2.30b) shows that the disorder renormalizations also have identical structure. In this sense, Eq. (2.28) confirms our previous result. In particular, it gives a microscopic derivation of how the electron-phonon coupling enters the disorder renormalization.<sup>11,10</sup> However, this "derivation" of the previous results was not quite honest. Even if one assumes  $\lambda$ ,  $\mu$ , and  $\hat{\rho}$  to be small,

of order  $\epsilon$ , say, the disorder corrections to  $\lambda$  and  $\mu$  are of  $O(\epsilon^2)$ , while those kept in Eqs. (3.1) are of  $O(\epsilon^3)$ , since  $f_2$  itself is of  $O(\epsilon^2)$ . Therefore, formally the effects considered in Ref. 10 have been of higher order than those neglected. In practice however, all the parameters are of  $O(1)$ , and the formal expansion arguments given above make little sense. The present self-consistent treatment of  $Y$  changes the perturbative result of Ref. 10  $1-f_2$ , into  $1/(1+f_2)$ , and the microscopic treatment of the attractive interaction yields  $\lambda \rightarrow \lambda f_1$ . Both effects counteract the  $T_c$  degradation. On the other hand, the  $f_2$  found here is considerably larger than that in the phenomenological approach. So we have two new effects counteracting each other. This is the reason why the results of Ref. 10 with phenomenological fit parameters  $\lambda$  and  $\mu$  were not a bad approximation to the present ones, as we will see below.

The renormalization  $\mu \rightarrow \mu f_3$  has been obtained before by Anderson *et al.*,<sup>8</sup> who additionally considered effects on  $\mu^*$  due to anomalous diffusion near an Anderson transition. In Ref. 9,  $f_3$  has been evaluated for the case of quasi-one-dimensional diffusion in a model for  $A-15$  materials. Keck and Schmid<sup>7</sup> considered a nondiffusion renormalization of  $\lambda$  different from what is described by our  $f_1$ . Within the general approximation scheme given in I, it corresponds to picking up the stress contributions to  $\alpha^2 F^F$  only. The diffusive Cooper-propagator renormalization expressed by  $f_1$  has not been considered before. Because of the diffusion pole, it is stronger than the stress renormalization. Evaluation of all renormalization functions up to stress contributions is possible, but already very cumbersome. Such a calculation would be necessary, although, to describe the  $T_c$  enhancement observed in weak-coupling materials.

### B. Comparison with experiment

Equation (2.28) can be directly compared with experiment. Unfortunately, there are not many data available for bulk materials, where  $T_c$  is given as a function of the resistivity. We have fitted our  $T_c$  formula to data on  $Nb_3Ge$ ,  $LuRh_4B_4$ , and  $ErRh_4B_4$  given by Rowell and Dynes in Ref. 5. We have assumed  $2k_F/\kappa=0.87$  (this yields  $\mu=0.37$ ,  $\xi=1.11$ ), and  $\Theta_D=300$  K for all materials. For  $Nb_3Ge$ , we have used the estimate  $\ln(E_B/\hbar\omega_0)=2$  obtained in Ref. 9 from band-structure considerations,  $\lambda=2.5$  and  $\rho_M=680 \mu\Omega$  cm. For the rare-earth rhodium bordies, we have chosen  $\ln(E_B/\hbar\omega_0)=5$  and  $\lambda=0.91$  (0.82),  $\rho_M=1400 \mu\Omega$  cm (1050  $\mu\Omega$  cm) for  $LuRh_4B_4$  ( $ErRh_4B_4$ ). The resulting fit is shown in Fig. 1. For  $\rho/\rho_M \leq 0.15$ , agreement is very good, while for larger resistivities (in the case of  $Nb_3Ge$ ) the observed  $T_c$  degradation is much stronger than that obtained from theory. We will come back to this discrepancy in the discussion below. For  $LuRh_4B_4$ , Rowell and Dynes<sup>5</sup> have also given data extending to larger resistivities. Figure 2 shows the best fit we could obtain with  $2k_F/\kappa=0.87$ ,  $\Theta_D=300$  K, and  $\ln(E_B/\hbar\omega_0)=5$ . We again have chosen  $\lambda=0.91$  and  $\rho_M=1400 \mu\Omega$  cm. As in the case of  $Nb_3Ge$ , agreement is very good for  $\rho/\rho_M \leq 0.15$ , while the theory cannot account for data at higher resistivities.

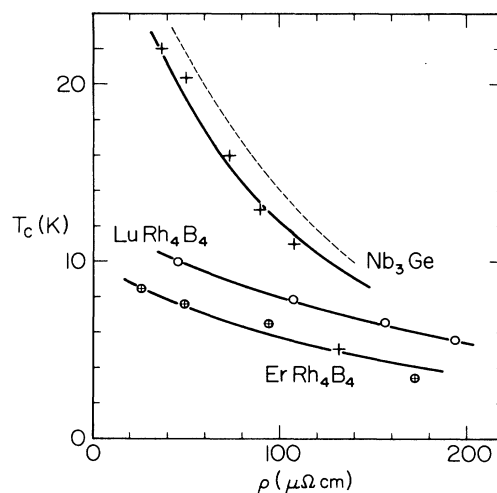


FIG. 1. Transition temperature versus resistivity for  $Nb_3Ge$  (crosses),  $LuRh_4B_4$  (circles), and  $ErRh_4B_4$  (crossed circles). Experimental data points have been redrawn from Ref. 5, Fig. 35. Solid lines represent the present theory with parameters as given in the text. The dashed line is the theoretical result for  $Nb_3Ge$  with magnetic-field-dependent terms removed, see text.

### C. Discussion

We first discuss the parameters used in the preceding section. The values for  $\mu$  and  $\xi$  are standard ones. Within  $\ln(E_B/\hbar\omega_0)=5$  they yield  $\mu^*=0.13$  at  $\rho=0$ , a common value for many materials.<sup>14</sup> As has been mentioned in Ref. 21,  $\lambda$  is a bare parameter which has no direct physical meaning for materials which do not have a

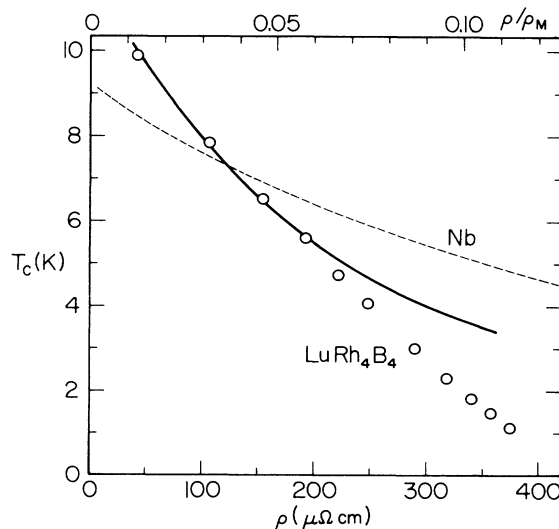


FIG. 2. Transition temperature versus resistivity for  $LuRh_4B_4$  (circles) and  $Nb$ . Data points have been redrawn from Ref. 5, Fig. 34. The solid line represents the fit of Eq. (2.28) to the data with parameters as given in the text. The dashed line is the theoretical prediction for  $Nb$ . The lower resistivity scale refers to  $LuRh_4B_4$ , the upper one to  $Nb$ .

clean limit. This is the case for  $\text{Nb}_3\text{Ge}$ , the value chosen corresponds to a clean limit  $T_c$  of 32.2 K. The Debye temperature chosen is the one for crystalline  $\text{Nb}_3\text{Ge}$ , and we have assumed the same value for the rare-earth rhodium borides. Little is known about variations of the Debye temperature with disorder, and we have assumed it to be constant. However, Tsuei<sup>23</sup> gives a value  $\Theta_D = 222$  K for amorphous  $\text{Nb}_3\text{Ge}$ . This indicates that there may be a significant drop of  $\Theta_D$  with disorder. Concurrently, one would expect a change in the phonon spectrum which determines the bare value of  $\lambda$ . The information presently available is not sufficient to take such effects into account. Another parameter is  $\ln(E_B/\hbar\omega_0)$ . For the rare-earth rhodium borides, we have used the common value of 5. For  $A$ -15's,  $\ln(E_B/\hbar\omega_0) = 2$  has been estimated in Ref. 9. Since this value is perhaps disputable, we have also tried  $\ln(E_B/\hbar\omega_0) = 5$  for  $\text{Nb}_3\text{Ge}$ . We then obtain a fit indistinguishable from the one shown in Fig. 1 with  $\lambda = 1.92$ ,  $\rho_M = 660 \mu\Omega \text{ cm}$ . The remaining parameter is the resistivity scale  $\rho_M$ . Although the values chosen are *a priori* reasonable, it is interesting that for  $\text{Nb}_3\text{Ge}$ , we need a value about half that for the rare-earth rhodium borides. In this context we note that all these materials show anomalies of the Mooij type<sup>24</sup> in the normal-state resistivity. For residual resistivities  $\rho_r$ , approaching a material dependent value  $\rho^*$ , the temperature coefficient of resistivity,  $\alpha = (1/\rho)d\rho/dT$ , gets smaller and smaller, and for  $\rho_r > \rho^*$ ,  $\alpha$  is negative. The high- $T_c$  superconductors share this behavior with a large number of other high-resistivity materials. There is no generally accepted explanation for this phenomenon. Recent proposals for an explanation include incipient Anderson localization,<sup>25</sup> phonon-induced tunneling,<sup>26</sup> and interaction anomalies.<sup>27</sup> All these explanations predict  $\rho^*$  to be proportional to  $\rho_M$ . From measurements of  $\rho$  versus  $T$  for the rare-earth rhodium borides,<sup>5</sup> we find  $\rho^* \simeq 280 \mu\Omega \text{ cm}$ , while for  $\text{Nb}_3\text{Ge}$  one has  $\rho^* = 100 \mu\Omega \text{ cm}$ .<sup>28</sup> This is consistent with our choices for  $\rho_M$ . We conclude that all parameters chosen for the fits are realistic.

In Ref. 5, data of  $T_c$  versus  $\rho$  for  $\text{Nb}_3\text{Sn}$  and  $\text{V}_3\text{Si}$  have also been given. Although the  $T_c$  degradation is of the same order of magnitude as for  $\text{Nb}_3\text{Ge}$ , the curves show a distinct *s* shape (especially for  $\text{Nb}_3\text{Sn}$ ). This cannot be explained by the present theory. We have speculated earlier<sup>10</sup> that band-structure effects may be important for these well-ordered, stoichiometric compounds, while in the metastable  $A$ -15's, such as  $\text{Nb}_3\text{Ge}$ , these effects are washed out, and can be neglected.

Let us come back to the failure of the theory at large resistivities. As has been emphasized in I, various approximations necessary to derive the strong-coupling equations restrict the validity of the theory to the regime  $\rho/\rho_M \ll 1$ . Therefore it is not surprising that we get significant deviations for  $\rho/\rho_M > 0.15$ . There are many effects which might play a role at higher resistivities, cf. the discussion in I. Presumably the most important one will be the disorder dependence of the dynamically screened Coulomb interaction, which has been neglected in our Thomas-Fermi approximation. Recent tunneling measurements<sup>29</sup> on aluminum approaching the metal-insulator transition indeed suggest that inelastic lifetime effects are the main

reason for the observed suppression of superconductivity. Although it would be very difficult to construct a complete theory in this regime, certain aspects of the disorder-dependent dynamical screening could be relatively easily taken into account within the framework provided in I. A first attempt to this direction has been made in Ref. 9. In this connection it is also interesting to note that the fits for the data shown in Figs. 1 and 2 obtained in Ref. 10 within a BCS-Bogoliubov theory were somewhat better at high resistivities. The technical reason is that in the perturbative treatment of Ref. 10, the normal self-energy yielded factors of  $(1 - \tilde{f}_2)$ , where  $\tilde{f}_2$  was slightly different from  $f_2$ . The present self-consistent treatment changes this into  $1/(1 + f_2)$ , as has been discussed in Sec. III A. As a consequence, the saturation tendency of  $T_c$  at large  $\rho$  is larger in the present formalism. However, in the region where this difference arises, the theory is not supposed to be valid anyway, as has been discussed above. For  $\rho/\rho_M \leq 0.15$ , the present theory provides a microscopic corroboration of the results obtained in Ref. 10 on the basis of a phenomenological model.

An extension of the formalism of Ref. 10 to finite magnetic fields revealed an interesting anomaly in the  $T$  dependence of  $H_{c2}$  at the critical point.<sup>30</sup> This effect was based on the fact that a magnetic field strongly weakens some contributions to the renormalization factors, viz., the Cooper-propagator renormalizations discussed at length in I. Since in the present theory new Cooper-propagator renormalizations are present, some of which tend to enhance  $T_c$ , one has to check whether the effect predicted in Ref. 30 survives. For this purpose we show in Fig. 1 as a dashed line, the result we obtain for  $\text{Nb}_3\text{Ge}$  by neglecting all Cooper-propagator renormalizations (with all other parameters kept fixed). The result shows that a magnetic field has an effect of the same sign and order of magnitude as in the BCS-Bogoliubov theory. So the prediction made in Ref. 30 for  $\text{Nb}_3\text{Ge}$  stands, although the numbers estimated may have been too optimistic by a factor of 2–3.

As we have discussed in the preceding section the parameters  $\lambda$  and  $\mu$  are clean-limit values. For the materials discussed so far, the clean limit does not exist, and so there is some freedom left in choosing  $\lambda$  and  $\mu$ . It would be very interesting to check Eq. (2.28) for a material which can be made very clean, and where  $\lambda$  and  $\mu$  are known. As an example, we choose Nb, for which the clean-limit McMillan solution has been designed. One has<sup>14</sup>  $\lambda = 0.82$ ,  $\Theta_D = 277$  K, and  $T_c(\rho = 0) = 9.2$  K. With  $\ln(E_B/\hbar\omega) = 5$ , this enforces  $2k_F/\kappa = 0.87$ . Under the assumption that these parameters do not change with disorder (which implies, e.g., that changes in the phonon spectrum are negligible) the only parameter left is  $\rho_M$ . The dotted line in Fig. 2 shows our prediction for Nb. Unfortunately, we could not find any data to compare with.

Finally, we emphasize that the present application of the theory presented in I still includes crude approximations. Even if one assumes the McMillan solution to be valid, the disorder parameters  $f_1$ ,  $f_2$ , and  $f_3$  have been evaluated by taking into account terms with diffusion enhancement only. In order to describe the less drastic effects observed in low- $T_c$  materials, it will be necessary to

improve at least on this point. This can be done by exploiting the general approximation scheme given in I. It will also be desirable to solve the equations numerically, at least the simplified version given in Sec. II, to check if the McMillan procedure is still reliable in the presence of disorder. These points are left for future investigations.

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- <sup>21</sup> $\lambda$  is a bare parameter which has a direct physical meaning only in the clean limit, which cannot always be realized experimentally. In this case,  $\lambda$  should not be taken as the values given in the literature by fitting the clean-limit McMillan formula to  $T_c$ . In such a procedure, some of the disorder effects calculated here have already been lumped into an effective value of  $\lambda$ .
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