COMBINED POTENTIAL AND SPIN IMPURITY SCATTERING IN CUPRATES*

G. Harań

Institute of Physics, Wrocław University of Technology
Wybrzeże Wyspiańskiego 27, 50-370 Wrocław, Poland

and A.D.S. Nagi

Department of Physics, University of Waterloo
Waterloo, Ontario, Canada, N2L 3G1

(Received June 21, 2001)

We present a theory of combined nonmagnetic and magnetic momentum-dependent impurity scattering in the d-wave superconductor. After deriving a formula for the initial suppression of the critical temperature we discuss the experimental data for Zn and Ni substitutions as well as electron irradiation defects in cuprates. We suggest, that the unequal pair-breaking effect of Zn and Ni may be related to a different structure of the magnetic moments induced by these impurities.

PACS numbers: 74.20.–z, 74.62.–c, 74.62.Dh, 74.72.–h

Unusual for the d-wave superconductivity in the disordered systems weak pair-breaking effect of impurities in cuprates [1–13] suggests, as a possible explanation, anisotropic impurity scattering [14–16]. Indeed, inclusion of non s-wave scattering channels in the impurity potential leads to a quantitative agreement of the theoretical predictions with the experimental data. In this paper, we generalize our former approach to a combined potential and magnetic impurity scattering. Such a study is motivated by the existence of a nontrivial magnetic structure of simple defects in cuprates. Residing in the magnetically active in-plane Cu ($3d^9$, $S = {}^1/_2$) sites the nominally nonmagnetic Zn ($3d^{10}$, $S = 0$) atoms induce the magnetic moments on the neighboring Cu sites [17–20] whereas the magnetic Ni ($3d^8$, $S = 1$) substitution

* Presented at the XII School of Modern Physics on Phase Transitions and Critical Phenomena, Lądek Zdrój, Poland, June 21–24, 2001.

results in a more localized screened impurity spin [19,20]. As indicated by macroscopic susceptibility and NMR measurements [17–19,21,22] the magnitude of the impurity-induced magnetic moments decreases with hole doping from $0.86\,\mu_{\rm B}$ for Zn, and $1.9\,\mu_{\rm B}$ for Ni in underdoped $YBa_2Cu_3O_{7-\delta}$ (Y-123) to $0.36\,\mu_{\rm B}$/Zn and $1.6\,\mu_{\rm B}$/Ni in the optimally doped system. In $La_{2-x}Sr_xCuO_4$ (La-214) the same impurity substitutions lead to magnetic properties corresponding to local magnetic moments of $1.0\,\mu_{\rm B}$/Zn and $0.6\,\mu_{\rm B}$/Ni [23]. Below, we discuss within the anisotropic impurity scattering scenario the pair-breaking effect of extended and localized impurity-induced magnetic moments in the d-wave superconductor.

We consider randomly distributed impurities at low concentration interacting with conduction electrons through a potential $u(\boldsymbol{k},\boldsymbol{k}') = v(\boldsymbol{k},\boldsymbol{k}') + J(\boldsymbol{k},\boldsymbol{k}')\bar{\boldsymbol{S}}\bar{\boldsymbol{\sigma}}$, where $\bar{\boldsymbol{S}}$ is a classical spin representing the impurity and $\bar{\boldsymbol{\sigma}}$ is the electron spin density. The potential in both nonmagnetic and magnetic channels is anisotropic and defined as

$$v\left(\boldsymbol{k},\boldsymbol{k}'\right) = v_{\rm i} + v_{\rm a} f\left(\boldsymbol{k}\right) f\left(\boldsymbol{k}'\right) , \tag{1}$$

$$J\left(\boldsymbol{k},\boldsymbol{k}'\right) = J_{\rm i} + J_{\rm a} f\left(\boldsymbol{k}\right) f\left(\boldsymbol{k}'\right) , \tag{2}$$

where $v_{\rm i}$ ($v_{\rm a}$), $J_{\rm i}$ ($J_{\rm a}$) are isotropic (anisotropic) scattering amplitudes in the nonmagnetic and magnetic scattering channel, respectively and $f\left(\boldsymbol{k}\right) = \pm 1$. The anisotropy function is chosen to vanish after averaging over the Fermi Surface (FS) momenta, *i.e.*, $\langle f \rangle = \int_{\rm FS} dS_k n(\boldsymbol{k}) f(\boldsymbol{k}) = 0$, where $n(\boldsymbol{k})$ is a normalized angle resolved FS density of states, $\int_{\rm FS} dS_k n(\boldsymbol{k}) = 1$. In addition, $f\left(\boldsymbol{k}\right)$ is normalized, such as $\langle f^2 \rangle = 1$. We use the above potential to simulate scattering potentials of Zn and Ni impurities in cuprate superconductors. A screened localized magnetic moment [19,20] of Ni corresponds to $J_{\rm a}/J_{\rm i} \ll 1$, while a broadly distributed over Cu sites Zn-induced magnetic moment [17–20] is approximated by $J_{\rm a}/J_{\rm i} \sim 1$, *i.e.*, comparable in magnitude scattering in both isotropic and anisotropic channels. We also assume that the nonmagnetic scattering represents the dominant contribution to the impurity potential and take $J_{\rm a}/v_{\rm a} < 1$, $J_{\rm i}/v_{\rm i} < 1$. Given the impurity potential we study its effect on the anisotropic superconducting state determined by the order parameter $\Delta(\boldsymbol{k}) = \Delta e(\boldsymbol{k})$, where $e\left(\boldsymbol{k}\right)$ is a momentum-dependent function normalized, such as $\langle e^2 \rangle = 1$. For the $d_{x^2-y^2}$-wave state $e(\boldsymbol{k}) = \sqrt{2}\cos 2\phi$ in a polar angle notation. Taking the electron-impurity scattering within the Born approximation and neglecting the impurity-impurity interaction, [24] the diagonal and off-diagonal corrections to the Green's function averaged over the impurity positions and spin orientations read [24,25]

$$\tilde{\omega}\left(\boldsymbol{k}\right) = \omega + \pi n_{\mathrm{i}} N_0 \int\limits_{\mathrm{FS}} dS_{\boldsymbol{k}'} n\left(\boldsymbol{k}'\right) \tilde{\omega}\left(\boldsymbol{k}'\right) \frac{\left[v^2\left(\boldsymbol{k},\boldsymbol{k}'\right) + J^2\left(\boldsymbol{k},\boldsymbol{k}'\right) S\left(S+1\right)\right]}{\left[\tilde{\omega}^2\left(\boldsymbol{k}'\right) + \tilde{\Delta}^2\left(\boldsymbol{k}'\right)\right]^{1/2}}, \tag{3}$$

$$\tilde{\Delta}\left(\boldsymbol{k}\right) = \Delta\left(\boldsymbol{k}\right) + \pi n_{\mathrm{i}} N_0 \int\limits_{\mathrm{FS}} dS_{\boldsymbol{k}'} n\left(\boldsymbol{k}'\right) \tilde{\Delta}\left(\boldsymbol{k}'\right) \frac{\left[v^2\left(\boldsymbol{k},\boldsymbol{k}'\right) - J^2\left(\boldsymbol{k},\boldsymbol{k}'\right) S\left(S+1\right)\right]}{\left[\tilde{\omega}^2\left(\boldsymbol{k}'\right) + \tilde{\Delta}^2\left(\boldsymbol{k}'\right)\right]^{1/2}}, \tag{4}$$

where $\omega = \pi T(2n+1)$ is the Matsubara frequency, T is the temperature, N_0 is the single-spin density of states at the Fermi level, and n_{i} is the impurity concentration. The self-energies (3), (4) are determined by $v^2\left(\boldsymbol{k},\boldsymbol{k}'\right)$ and $J^2\left(\boldsymbol{k},\boldsymbol{k}'\right)$ which according to definition (1) read

$$v^2\left(\boldsymbol{k},\boldsymbol{k}'\right) = v_0^2 \pm v_1^2 f\left(\boldsymbol{k}\right) f\left(\boldsymbol{k}'\right), \tag{5}$$

$$J^2\left(\boldsymbol{k},\boldsymbol{k}'\right) = J_0^2 \pm J_1^2 f\left(\boldsymbol{k}\right) f\left(\boldsymbol{k}'\right), \tag{6}$$

where $v_0^2 = v_{\mathrm{i}}^2 + v_{\mathrm{a}}^2$, $v_1^2 = 2|v_{\mathrm{i}} v_{\mathrm{a}}|$, $J_0^2 = J_{\mathrm{i}}^2 + J_{\mathrm{a}}^2$, and $J_1^2 = 2|J_{\mathrm{i}} J_{\mathrm{a}}|$. Note that $v_1^2 \leq v_0^2$ and $J_1^2 \leq J_0^2$. Before proceeding further, we introduce the intrinsic scattering rates $\Gamma_0 = \pi n_{\mathrm{i}} N_0 v_0^2$, $\Gamma_1 = \pm \pi n_{\mathrm{i}} N_0 v_1^2$, $G_0 = \pi n_{\mathrm{i}} N_0 J_0^2 S\left(S+1\right)$, and $G_1 = \pm \pi n_{\mathrm{i}} N_0 J_1^2 S\left(S+1\right)$. It is easy to see that $-1 \leq \Gamma_1/\Gamma_0 \leq 1$ and $-1 \leq G_1/G_0 \leq 1$. We use the above parameters to simulate the magnetic structure of scattering centers. The Zn-induced extended magnetic moment is defined by $G_1/G_0 \sim 1$ while the localized moment generated by Ni substitution is determined by $G_1/G_0 \ll 1$. Taking a separable pair potential $V\left(\boldsymbol{k},\boldsymbol{k}'\right) = -V_0 e\left(\boldsymbol{k}\right) e\left(\boldsymbol{k}'\right)$, $V_0 > 0$, and following a standard procedure [14,25] we obtain the critical temperature, T_{c}, equation

$$\begin{aligned} \ln \frac{T_{\mathrm{c}}}{T_{\mathrm{c}0}} = {} & \left(1 - \langle e\rangle^2 - \langle ef\rangle^2\right) \left[\psi\left(\frac{1}{2}\right) - \psi\left(\frac{1}{2} + \frac{\Gamma_0 + G_0}{2\pi T_{\mathrm{c}}}\right)\right] \\ & + \langle ef\rangle^2 \left[\psi\left(\frac{1}{2}\right) - \psi\left(\frac{1}{2} + \frac{\Gamma_0 + G_0 + G_1 - \Gamma_1}{2\pi T_{\mathrm{c}}}\right)\right] \\ & + \langle e\rangle^2 \left[\psi\left(\frac{1}{2}\right) - \psi\left(\frac{1}{2} + \frac{2G_0}{2\pi T_{\mathrm{c}}}\right)\right], \end{aligned} \tag{7}$$

where $T_{\mathrm{c}0}$ is the critical temperature in the absence of impurities. Comparing the above equation with the one for nonmagnetic scattering (Eq. (24) of Ref. [14]) we notice that the spin-flip scattering manifests in Eq. (7) through a single term determined by the exchange rate $2G_0$. The remaining terms

correspond to the ones obtained for potential scattering [14] with some new effective scattering rates being combinations of the scattering rates in the magnetic and nonmagnetic channels: $\bar{\Gamma}_0 = \Gamma_0 + G_0, \bar{\Gamma}_1 = \Gamma_1 - G_1$. The role of anisotropy in the impurity potential is expressed by the dimensionless parameter $\langle ef \rangle^2$ which is positive and does not exceed the Fermi surface average of the absolute value of the order parameter $\langle |e| \rangle^2$. For the d-wave state and a cylindrical Fermi surface $\langle |e| \rangle^2 \simeq 0.81$. In the quantitative analysis of the experimental data we consider the T_c reduction in the limit of low impurity concentration $n_i \to 0$ which is determined by the initial slope

$$\frac{dT_c}{d\rho_0} \simeq -0.614\, \omega_{pl}^2 \left[\chi + (1-\chi)\,\phi_M - \phi_A\right] K/\,\mu\Omega\mathrm{cm}\,, \tag{8}$$

where ρ_0 is the residual resistivity at the zero frequency, [14] and ω_{pl} is the in-plane plasma frequency in eV. For the sake of brevity we have also introduced $\chi = 1 - \langle e \rangle^2$, $\phi_A = \langle ef \rangle^2 \bar{\Gamma}_1/\bar{\Gamma}_0$ (anisotropy factor), and $\phi_M = 2G_0/\bar{\Gamma}_0$ (magnetic factor). We find that in the d-wave state ($\chi = 1$) the initial T_c suppression (8) is determined solely by the dimensionless anisotropy factor ϕ_A. The influence of the spin-flip scattering is present through the renormalized scattering rates in the isotropic and anisotropic scattering channels: $\bar{\Gamma}_0$ and $\bar{\Gamma}_1$. In Tables I–III we give the anisotropy factors ϕ_A needed to account for the experimental data of Zn, Ni and oxygen vacancy-induced T_c suppression in Y-123, La-214 and Bi-2212 compounds. Except for Ni effect in overdoped Y-123 films (Ref. [12]) the anisotropy factor does not exceed the maximal allowed value of 0.81. Worth noting are significantly lower values of ϕ_A for Zn substitution than those for Ni. This feature can be attributed to a different nature of the magnetic moments associated with these impurities. While the Zn-induced moment is broadly distributed over neighboring Cu sites, $G_1/G_0 \sim 1$, the one created by Ni is screened on a larger distance and is more localized $G_1/G_0 \ll 1$. Therefore, for comparable amounts of isotropic scattering by these impurities [26], $\bar{\Gamma}_0 = \Gamma_0 + G_0$, the anisotropy factor $\phi_A \sim (\Gamma_1 - G_1)\,/\,(\Gamma_0 + G_0)$ of Ni scattering potential should exceed the one of Zn impurity. The above analysis depends on the relative magnitude of the magnetic to nonmagnetic scattering. Therefore, to decide definitely about the role of spin scattering in high temperature superconductors with simple defects a quantitative estimate of the rates G_0/Γ_0 and G_1/Γ_1 is needed.

Concluding, we find that even in the presence of the spin-flip processes the scenario of anisotropic impurity scattering accounts quantitatively for the experimentally observed T_c suppression due to Zn, Ni and oxygen vacancy scattering. Moreover, a different partition of the magnetic scattering rates into isotropic and anisotropic scattering channels can be used in the interpretation of the weak Ni-induced and relatively strong Zn-induced pair-breaking.

TABLE I

Y-123: ϕ_A anisotropy factor of the impurity potential reproducing the T_c suppression in the Y-123 compound within the d-wave superconductivity scenario, *i.e.*, $\chi = 1$. ($1.1\,\text{eV} \leq \omega_{pl} \leq 1.4\,\text{eV}$; ov. = overdoped, op. = optimally doped, un. = underdoped).

Defect	Sample	$\left(\frac{dT_c}{d\rho_0}\right)_{exp}$ [K/$\mu\Omega$ cm]	Anisotropy factor: ϕ_A
Zn impurity	(ov.) single crystal [5]	-0.674	$0.093 \leq \phi_A \leq 0.440$
	(ov.) single crystal [6,9]	-0.57	$0.233 \leq \phi_A \leq 0.526$
	(op.) thin film [10]	-0.241	$0.676 \leq \phi_A \leq 0.780$
	(op.) thin film [11]	-0.520	$0.300 \leq \phi_A \leq 0.568$
Ni impurity	(ov.) ceramic sample [9]	-0.333	$0.552 \leq \phi_A \leq 0.723$
	(ov.) film [12]	$(-0.063) \div (-0.044)$	$0.915 \leq \phi_A \leq 0.963$
oxygen vacancy	(ov.) single crystal [2]	-0.30 ± 0.04	$0.542 \leq \phi_A \leq 0.784$
	(ov.) film [1]	-0.187	$0.748 \leq \phi_A \leq 0.845$

TABLE II

La-214: ϕ_A anisotropy factor of the impurity potential reproducing the T_c suppression in the La-214 compound within the d-wave superconductivity scenario, *i.e.*, $\chi = 1$. ($\omega_{pl} = 0.84$ eV; notation as in Table I.)

Defect	Sample	$\left(\frac{dT_c}{d\rho_0}\right)_{exp}$ [$K/\mu\Omega$ cm]	Anisotropy factor: ϕ_A
Zn impurity	(ov.) single crystal [6]	-0.37	0.146
	(un.) film [7,8]	-0.233	0.462
oxygen vacancy	(un.) film [3]	-0.127	0.707

TABLE III

Bi-2212: ϕ_A anisotropy factor of the impurity potential reproducing the T_c suppression in the Bi-2212 compound within the d-wave superconductivity scenario, *i.e.*, $\chi = 1$. ($\omega_{pl} = 0.9$ eV; notation as in Table I.)

Defect	Sample	$\left(\frac{dT_c}{d\rho_0}\right)_{exp}$ [$K/\mu\Omega$ cm]	Anisotropy factor: ϕ_A
oxygen vacancy	(ov.) single crystal [4]	-0.28	0.437

The work was supported in part by the Polish State Committee for Scientific Research (KBN) grant No. 5P03B05820.

REFERENCES

[1] S. Tolpygo, J.-Y. Lin, M. Gurvitch, S.Y. Hou, J.M. Philips, *Phys. Rev.* **B53**, 12454 (1996); **B53**, 12462 (1996).

[2] J. Giapintzakis, D.M. Ginsberg, M.A. Kirk, S. Ockers, *Phys. Rev.* **B50**, 15967 (1994).

[3] K. Karpińska, private communication.

[4] F. Rullier-Albenque, A. Legris, H. Berger, L. Forro, *Physica* **C254**, 88 (1995).

[5] T.R. Chien, Z.Z. Wang, N.P. Ong, *Phys. Rev. Lett.* **67**, 2088 (1991).

[6] Y. Fukuzumi, K. Mizuhashi, K. Takenaka, S. Uchida, *Phys. Rev. Lett.* **76**, 684 (1996).

[7] M.Z. Cieplak, K. Karpińska, J. Domagała, E. Dynowska, M. Berkowski, A. Malinowski, S. Guha, M. Croft, P. Lindenfeld, *Appl. Phys. Lett.* **73**, 2823 (1998).

[8] K. Karpińska, M.Z. Cieplak, S. Guha, A. Malinowski, T. Skośkiewicz, W. Plesiewicz, M. Berkowski, B. Boyce, T.R. Lemberger, P. Lindenfeld, *Phys. Rev. Lett.* **84**, 155 (2000).

[9] Y. Zhao, H.K. Liu, G. Yang, S.X. Dou, *J. Phys. Condens. Matter* **5**, 3623 (1993).

[10] J. Schroeder, M. Ye, J.F. de Marneffe, M. Mehbod, R. Deltour, A.G.M. Jansen, P. Wyder, *Physica* **C278**, 113 (1997).

[11] D.J.C. Walker, A.P. Mackenzie, J.R. Cooper, *Phys. Rev.* **B51**, 15653 (1995).

[12] J.-T. Kim, D.G. Xenikos, A. Thorns, T.R. Lemberger, *J. Appl. Phys.* **72**, 803 (1992).

[13] R.J. Radtke, K. Levin, H.-B. Schüttler, M.R. Norman, *Phys. Rev.* **B48**, 653 (1993).

[14] G. Harań, A.D.S. Nagi, *Phys. Rev.* **B54**, 15463 (1996).

[15] G. Harań, A.D.S. Nagi, *Solid State Commun.* **106**, 775 (1998).

[16] G. Harań, A.D.S. Nagi, *Phys. Rev.* **B58**, 12441 (1998).

[17] A.V. Mahajan, H. Alloul, G. Collin, J.F. Marucco, *Phys. Rev. Lett.* **72**, 3100 (1994).

[18] G.V. Williams, J.L. Tallon, R. Meinhold, *Phys. Rev.* **B52**, 7034 (1995).

[19] J. Bobroff, H. Alloul, Y. Yoshinari, A. Keren, P. Mendels, N. Blanchard, G. Collin, J.-F. Marucco, *Phys. Rev. Lett.* **79**, 2117 (1997); *Physica* **C282-287**, 1389 (1997).

[20] R. Kilian, S. Krivenko, G. Khaliullin, P. Fulde, *Phys. Rev.* **B59**, 14432 (1999).

[21] P. Mendels, H. Alloul, G. Collin, N. Blanchard, J.F. Marucco, J. Bobroff, *Physica* **C235-240**, 1595 (1994).

[22] T.M. Riseman, H. Alloul, A.V. Mahajan, P. Mendels, N. Blanchard, G. Collin, J.F. Marucco, *Physica* **C235-240**, 1593 (1994).

[23] G. Xiao, M.Z. Cieplak, J.Q. Xiao, C.L. Chien, *Phys. Rev.* **B42**, 8752 (1990).

[24] A.A. Abrikosov, L.P. Gorkov, *Zh. Eksp. Teor. Fiz.* **39**, 1781 (1960) [*Sov. Phys. JETP* **12**, 1243 (1961)].

[25] K. Maki, in *Superconductivity*, ed. R.D. Parks, Marcel Dekker, New York 1969, Vol. 2, pp. 1035-1102.

[26] There is still no complete experimental agreement on the impurity-induced resistivity in the cuprates (Refs. [5, 6, 9, 11, 12]). Nevertheless, some results (Refs. [5, 9]) suggest a comparable effect of Zn and Ni impurities.