Disorder-induced transition between $s_\pm$ and s_{++} states in two-band superconductors

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We have reexamined the problem of disorder in two-band superconductors, and shown, within the framework of the T-matrix approximation, that the suppression of T_c can be described by a single parameter depending on the intraband and interband impurity scattering rates. T_c is shown to be more robust against nonmagnetic impurities than would be predicted in the trivial extension of Abrikosov-Gor'kov theory. We find a disorder-induced transition from the $s_\pm$ state to a gapless and then to a fully gapped s_{++} state, controlled by a single parameter—the sign of the average coupling constant $\langle\lambda\rangle$. We argue that this transition has strong implications for experiments.

Introduction. The symmetry and structure of the superconducting order parameter in recently discovered iron-based superconductors (FeSC) is one of the main challenges in this field.[1] The Fermi surface (FS) is usually given by two small hole pockets around the $\Gamma = (0,0)$ point and two electron pockets around the $M = (\pi,\pi)$ point in the 2-Fe Brillouin zone. The proximity of the competing spin-density-wave (SDW) state with $\mathbf{Q} = (\pi,\pi)$ suggests antiferromagnetic fluctuations as a mechanism for electron pairing. In this case, the natural order parameter for most of the FeSC is the so-called $s_\pm$ state, described by an isotropic order parameter on each FS with the opposite signs for electronlike and holelike pockets. Many experimental results, such as the NMR spin-lattice relaxation rate, the spin-resonance peak at the SDW wave vector $\mathbf{Q}$ in inelastic neutron scattering, and quasiparticle interference in tunneling experiments, are in good qualitative agrement with this scenario, although some materials are more anisotropic than others.[2]

Since varying amounts of disorder are present in the materials, and because superconductivity is created in some cases by doping, it is important to understand the role of impurities. It has been shown that in an $s_\pm$ state, any nonmagnetic impurity which scatters *solely* between the bands with a different sign of the order parameter suppresses T_c in the same way as a magnetic impurity in a single-band BCS superconductor.[3] Therefore, the critical temperature T_c should obey the Abrikosov-Gor'kov (AG) formula $\ln T_{c0}/T_c = \Psi(1/2 + \Gamma/2\pi T_c) - \Psi(1/2)$, where $\Psi(x)$ is the digamma function and T_{c0} is the critical temperature in the absence of impurities.[4] The critical value of the scattering rate Γ defined by $T_c(\Gamma^{\rm crit}) = 0$ is given by $\Gamma^{\rm crit}/T_{c0} = \pi/2\gamma \approx 1.12$ within AG theory. However, in several experiments on FeSC, e.g., Zn substitution or proton irradiation, it is found[5–8] that the T_c suppression is much less than expected in the framework of AG theory. It has therefore been suggested that the $s_\pm$ state is not realized at all in these systems, and that a more conventional two-band order parameter without sign change (s_{++}) is the more likely ground state.[9,10]

The disorder problem in these systems is substantially more complicated than this simple argument suggests, however. Even within the assumption of isotropic gaps on two different Fermi pockets and nonmagnetic scattering, a much slower pair-breaking rate can be achieved by assuming that the scattering is primarily intraband rather than interband. In the pure intraband scattering limit, Anderson's theorem applies, the system is insensitive to the sign of the order parameter, and no T_c suppression occurs. The rate of T_c suppression therefore apparently depends on the interplay of both intraband and interband scattering rates, and drawing conclusions regarding the superconducting state based on systematic disorder studies is fundamentally more difficult than in one-band systems. One approach to this problem has been to try to determine the intraband and interband scattering potentials microscopically for each type of impurity and host,[11–13] but the quantitative applicability of band theory to such questions is unclear.

Here we consider the critical temperature of an isotropic $s_\pm$ two-band superconductor within the usual self-consistent T-matrix approximation for impurity scattering.[14] We perform the study both analytically in the weak-coupling regime and numerically in the strong-coupling Eliashberg framework. We find that the dependence of T_c on impurity concentration is given by a universal form independent of impurity potentials, with respect to a generalized pair-breaking parameter. The form depends, however, on the ratio of interband to intraband pairing matrix elements. Depending on the average values of these matrix elements, we find there are two possible types of $s_\pm$ superconductivity. The first is the one which has been largely discussed so far in the literature, for which T_c is suppressed as disorder is increased, until it vanishes at a critical value of the scattering rate. There is, however, also a second type of $s_\pm$ state, one for which T_c tends to a finite value as disorder increases; at the same time the gap function acquires a uniform sign, i.e., undergoes a transition from $s_\pm$ to s_{++}.

Model. We consider the Eliashberg equations[14] for a two-band superconductor with a 4×4 matrix quasiclassical Green's function in Nambu and band space,

$$\hat{\mathbf{g}}(\omega_n) = \begin{pmatrix} g_{0a} & 0 \\ 0 & g_{0b} \end{pmatrix} \otimes \hat{\tau}_0 + \begin{pmatrix} g_{1a} & 0 \\ 0 & g_{1b} \end{pmatrix} \otimes \hat{\tau}_2, \quad (1)$$

where the τ_i denote Pauli matrices in Nambu space, and $g_{0\alpha}$ and $g_{1\alpha}$ are the normal and anomalous ξ-integrated Nambu Green's functions:

$$g_{0\alpha} = -\frac{i\pi N_\alpha \tilde{\omega}_{\alpha n}}{\sqrt{\tilde{\omega}_{\alpha n}^2 + \tilde{\phi}_{\alpha n}^2}}, \quad g_{1\alpha} = -\frac{\pi N_\alpha \tilde{\phi}_{\alpha n}}{\sqrt{\tilde{\omega}_{\alpha n}^2 + \tilde{\phi}_{\alpha n}^2}}. \quad (2)$$

Here, index α runs over band indices a and b, $N_{a,b}$ are the density of states of each band (a, b) at the Fermi level, and $\omega_n = \pi T(2n+1)$ is the Matsubara frequency. The quantities $\tilde{\omega}_{\alpha n}$ and $\tilde{\phi}_{\alpha n}$ are Matsubara frequencies and order parameters renormalized by the self-energy $\hat{\Sigma}(i\omega_n)$, respectively,

$$\tilde{\omega}_{\alpha n} = \omega_n + i\Sigma_{0\alpha}(i\omega_n) + i\Sigma_{0\alpha}^{\mathrm{imp}}(i\omega_n), \quad (3)$$

$$\tilde{\phi}_{\alpha n} = \Sigma_{1\alpha}(i\omega_n) + \Sigma_{1\alpha}^{\mathrm{imp}}(i\omega_n). \quad (4)$$

The self-energy due to the spin fluctuation interaction is then given by

$$\Sigma_{0\alpha}(i\omega_n) = T\sum_{\omega_n',\beta} |\lambda_{\alpha\beta}(n-n')| g_{0\beta}/N_\beta, \quad (5)$$

$$\Sigma_{1\alpha}(i\omega_n) = -T\sum_{\omega_n',\beta} \lambda_{\alpha\beta}(n-n') g_{1\beta}/N_\beta. \quad (6)$$

The coupling functions $\lambda_{\alpha\beta}(n-n') = 2\lambda_{\alpha\beta}\int_0^\infty d\Omega\, \Omega B(\Omega)/[(\omega_n - \omega_{n'})^2 + \Omega^2]$ are expressed via the spectral functions $B(\Omega)$ (Ref. 15) and constants $\lambda_{\alpha\beta}$. The matrix elements $\lambda_{\alpha\beta}$ can be positive (attractive) as well as negative (repulsive) due to the interplay between spin fluctuations and electron-phonon coupling[15,16] and strongly renormalized due to the nested Coulomb interaction.[17]

We use the T-matrix approximation to calculate the average impurity self-energy $\hat{\Sigma}^{\mathrm{imp}}$:

$$\hat{\Sigma}^{\mathrm{imp}}(i\omega_n) = n_{\mathrm{imp}}\hat{U} + \hat{U}\hat{g}(\omega_n)\hat{\Sigma}^{\mathrm{imp}}(i\omega_n), \quad (7)$$

where $\hat{U} = U \otimes \hat{\tau}_3$ and n_{imp} is impurity concentration. For simplicity, intraband and interband parts of the potential are set equal to v and u, respectively, such that $(U)_{\alpha\beta} = (v - u)\delta_{\alpha\beta} + u$. This completes the specification of the equations which determine the quasiclassical Green's functions.

Note that we have neglected possible anisotropy in each order parameter $\tilde{\phi}_{a(b)n}$; these effects can lead to changes in the response of the two-band $s_\pm$ system to disorder and have been examined, e.g., in Ref. 18.

Critical temperature. T_c is found by solving the linearized Eliashberg equations for the renormalization factors $\tilde{Z}_{\alpha n} = \tilde{\omega}_{\alpha n}/\omega_n$ and gap functions $\tilde{\Delta}_{\alpha n} = \tilde{\phi}_{\alpha n}/\tilde{Z}_{\alpha n}$:[14]

$$\tilde{Z}_{\alpha n} = 1 + \sum_\beta \tilde{\Gamma}_{\alpha\beta}/|\omega_n|$$
$$+ \pi T_c \sum_{\omega_n',\beta} |\lambda_{\alpha\beta}(n-n')|\mathrm{sgn}(\omega_{n'})/\omega_n, \quad (8)$$

$$\tilde{Z}_{\alpha n}\tilde{\Delta}_{\alpha n} = \sum_\beta \tilde{\Gamma}_{\alpha\beta}\tilde{\Delta}_{\beta n}/|\omega_n|$$
$$+ \pi T_c \sum_{\omega_n',\beta} \lambda_{\alpha\beta}(n-n')\tilde{\Delta}_{\beta n'}/|\omega_{n'}|, \quad (9)$$

where $\tilde{\Gamma}_{\alpha\beta}$ are impurity scattering rates.

If one inserts Eq. (8) into Eq. (9) and gets a set of equations for $\tilde{\Delta}_{\alpha n}$, it is easy to show that the impurity intraband scattering terms $\propto \tilde{\Gamma}_{aa}$ and $\tilde{\Gamma}_{bb}$ drop out,[19] in agreement with Anderson's theorem. From Eq. (7) one finds $\tilde{\Gamma}_{ab(ba)}$ as

$$\tilde{\Gamma}_{ab(ba)} = \Gamma_{a(b)}\frac{(1-\tilde{\sigma})}{\tilde{\sigma}(1-\tilde{\sigma})\eta\frac{(N_a+N_b)^2}{N_aN_b} + (\tilde{\sigma}\eta - 1)^2}, \quad (10)$$

where $\tilde{\sigma} = (\pi^2 N_a N_b u^2)/(1 + \pi^2 N_a N_b u^2)$ and $\Gamma_{a(b)} = n_{\mathrm{imp}}\pi N_{b(a)}u^2(1-\tilde{\sigma})$ are generalized cross-section and normal-state scattering rate parameters, respectively. The parameter η controls the ratio of intraband and interband scattering as $v^2 = u^2\eta$. In the *Born*(weak scattering) *limit*, $\tilde{\sigma} \to 0$, while for $\tilde{\sigma} \to 1$ the *unitary limit* (strong scattering) is achieved. From (10), we therefore recover explicitly the well-known but counterintuitive result that in the unitary limit nonmagnetic impurities do not affect T_c in an $s_\pm$ state.[19,20]

The linearized Eliashberg equations (8) and (9) are now solved numerically, varying T and finding T_c as the highest temperature where a nontrivial solution appears. Results for T_c as a function of $\tilde{\Gamma}_{ab}$, are shown in Fig 1, in which situation all cases with various values of $\tilde{\sigma}$ and η fall on the same universal T_c curve for each average $\langle\lambda\rangle \equiv [(\lambda_{aa} + \lambda_{ab})N_a/N + (\lambda_{ba} + \lambda_{bb})N_b/N]$ with $N = N_a + N_b$. It is clearly seen that depending on the sign of $\langle\lambda\rangle$, one gets two types of T_c behavior versus $\tilde{\Gamma}_{ab}$ in the $s_\pm$ scenario. For type (i), the critical temperature vanishes at a finite impurity scattering rate Γ_a^{crit} for $\langle\lambda\rangle < 0$. For type (ii), $\langle\lambda\rangle > 0$, the critical temperature remains finite at $\Gamma_a \to \infty$. In the marginal case of $\langle\lambda\rangle = 0$ we find that $\tilde{\Gamma}^{\mathrm{crit}} \to \infty$ but with exponentially small T_c. Therefore, we have found universal behavior of T_c controlled by a single parameter $\langle\lambda\rangle$.

Weak-coupling limit. To understand the origin of the two types of limiting behavior of T_c in an $s_\pm$ scenario, we now consider the weak-coupling limit assuming $\lambda_{\alpha\beta}(n-n') = \lambda_{\alpha\beta}\Theta(\omega_0 - |\omega_n|)\Theta(\omega_0 - |\omega_n'|)$. In this approximation the calculation can be performed analytically.
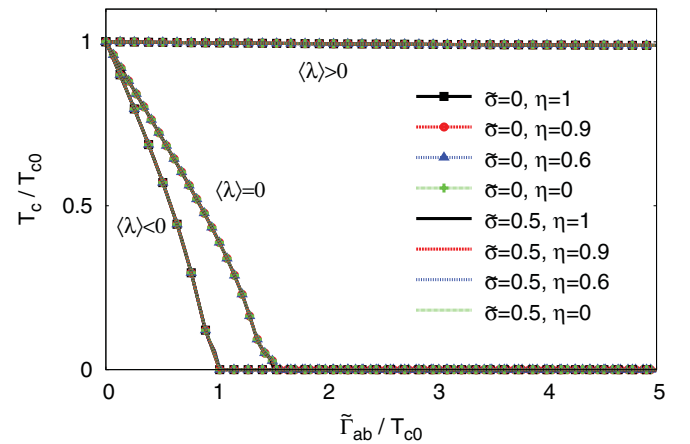

FIG. 1. (Color online) Critical temperature for various $\tilde{\sigma}$ and η as a function of the effective interband scattering rate $\tilde{\Gamma}_{ab}$ for the same parameters. Note that curves for different sets of $\tilde{\sigma}$ and η overlap and fall onto one of the three universal curves depending on the $\langle\lambda\rangle$. $N_b/N_a = 2$, coupling constants for illustrative purpose are chosen for $\langle\lambda\rangle > 0$ as $(\lambda_{aa},\lambda_{ab},\lambda_{ba},\lambda_{bb}) = (3,-0.2,-0.1,0.5)$, for $\langle\lambda\rangle = 0$ as $(2,-2,-1,1)$, and for $\langle\lambda\rangle < 0$ as $(1,-2,-1,1)$.

We introduce the parameter

$$\Delta_\alpha = \Theta(\omega_0 - |\omega_n|) \sum_\beta \lambda_{\alpha\beta} \pi T \sum_{|\omega_n| < \omega_0} \frac{\tilde{\Delta}_{\beta n}}{|\omega_n|}, \quad (11)$$

which plays the role of the pair potential in the clean limit. Substituting $\tilde{\Delta}_{\alpha n}$ from Eqs. (8) and (9) and recalling $\tilde{\Gamma}_{ab}/\tilde{\Gamma}_{ba} = N_b/N_a$, we get for $|\omega_n| < \omega_0$ an equation for Δ_α similar to AG:

$$\Delta_\alpha = \lambda_\alpha \langle \Delta \rangle (I_1 - I_2) + I_2 \sum_\beta \lambda_{\alpha\beta} \Delta_\beta, \quad (12)$$

where $I_1 = \pi T \sum_{|\omega_n| < \omega_0} 1/|\omega_n| \approx \log 2\gamma \omega_0/(\pi T_c)$, $I_2 = \pi T \sum_{|\omega_n| < \omega_0} 1/(|\omega_n| + \tilde{\Gamma}_{ab} + \tilde{\Gamma}_{ba})$, $\lambda_\alpha = \sum_\beta \lambda_{\alpha\beta}$, and $\langle \Delta \rangle = (\Delta_a N_a/N + \Delta_b N_b/N)$.

In the clean limit $I_2 = I_1$, Eq. (12) reduces to $\Delta_\alpha = I_1 \sum_\beta \lambda_{\alpha\beta} \Delta_\beta$. Diagonalization of this equation results in the equation for the critical temperature $I_1 = 1/\lambda_0$, where $\lambda_0 = (\lambda_{aa} + \lambda_{bb})/2 + \sqrt{(\lambda_{aa} - \lambda_{bb})^2/4 + \lambda_{ab}\lambda_{ba}} > 0$ is the highest positive eigenvalue of the matrix $\lambda_{\alpha\beta}$. The critical temperature is then $T_{c0} = \frac{2\gamma}{\pi}\omega_0 \exp(-1/\lambda_0)$. A similar expression was found in Refs. 3 and 21. The relative sign of the pair potential of the bands is determined by the off-diagonal interaction matrix elements: $\mathrm{sgn}(\Delta_a/\Delta_b) = \mathrm{sgn}(\lambda_{ab})$.

When $\Delta_a - \Delta_b \neq 0$, nonmagnetic impurities suppress the critical temperature.[3] The critical value of the impurity scattering rate for type (i) systems is given by $\ln[\omega_0/(\tilde{\Gamma}_{ab} + \tilde{\Gamma}_{ba})_{\mathrm{crit}}] = \langle \lambda \rangle/(\lambda_{aa}\lambda_{bb} - \lambda_{ab}\lambda_{ba})$.

We now focus on the case of type (ii) systems $\langle \lambda \rangle > 0$, which, to the best of our knowledge, have not been discussed extensively in the literature. Multiplying both sides of Eq. (12) with N_α, followed by a summation and using in the dirty limit $I_2 \to 0$, one obtains $1 = I_1\langle \lambda \rangle$ and consequently $T_c = \frac{2\gamma}{\pi}\omega_0 \exp(-1/\langle \lambda \rangle)$. Analysis of Eqs. (8) and (9) shows that, for small n in the clean limit, $\tilde{\Delta}_{\alpha n} \sim \Delta_\alpha$, while in the dirty limit both $\tilde{\Delta}_{an}$ and $\tilde{\Delta}_{bn}$ converge to the same value, $\tilde{\Delta}_{\alpha n} \to \Delta_{\Gamma \to \infty}$, that is, the s_{++} state is realized. If the initial state corresponds to $s_\pm$, a transition $s_\pm \to s_{++}$ at a finite concentration of impurities must exist.

There is a simple physical argument behind the $s_\pm \to s_{++}$ transition. With increasing interband disorder, the gap functions on the different Fermi surfaces tend to the same value. A similar effect has been found in Refs. 3 and 22 for a two-band systems with s_{++} symmetry, and in Ref. 18 discussing node lifting on the electron pockets for the extended s-wave state in FeSC.

To demonstrate the transition explicitly, we calculate $\tilde{\Delta}_{\alpha n}$ for $n = 0, 1, 2$ at $T = 0.04T_{c0}$ and show the results in Fig. 2 for a particular choice of $\lambda_{\alpha\beta}$ with $\langle \lambda \rangle > 0$. For this parameter set, $T_{c0} \approx 40$ K. Both order parameters $\tilde{\Delta}_{a(b)n}$ converge to $\Delta_{\Gamma \to \infty}$ for large disorder, while the T_c suppression quickly saturates. The transition $s_\pm \to s_{++}$ provides a possible explanation for the observed much weaker reduction of the critical temperature than the naive application of the AG formula.

Another important consequence of the transition $s_\pm \to s_{++}$, relevant to experiments in pnictides, is gapless superconductivity as one of the gaps vanishes. The density of states $N_{\mathrm{tot}}(\omega) = -\sum_\alpha \mathrm{Im}\, g_{0\alpha}(\omega)/\pi$ is shown in Fig. 3(a) for a type (ii) case. With increasing impurity scattering rate,
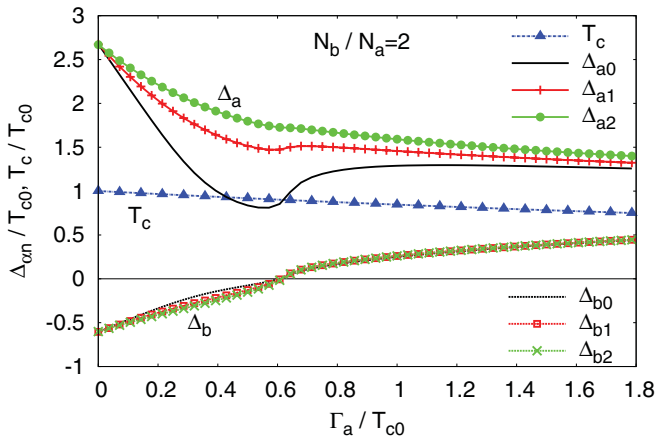

FIG. 2. (Color online) Critical temperature T_c and $\tilde{\Delta}_{\alpha n}$ (in units of T_{c0}) for first, second, and third Matsubara frequencies n at $T = 0.04T_{c0}$, $\tilde{\sigma} = 0.5$, $\eta = 1$, and $N_b/N_a = 2$ and $\langle \lambda \rangle > 0$. The coupling constants are chosen as in Fig. 1.
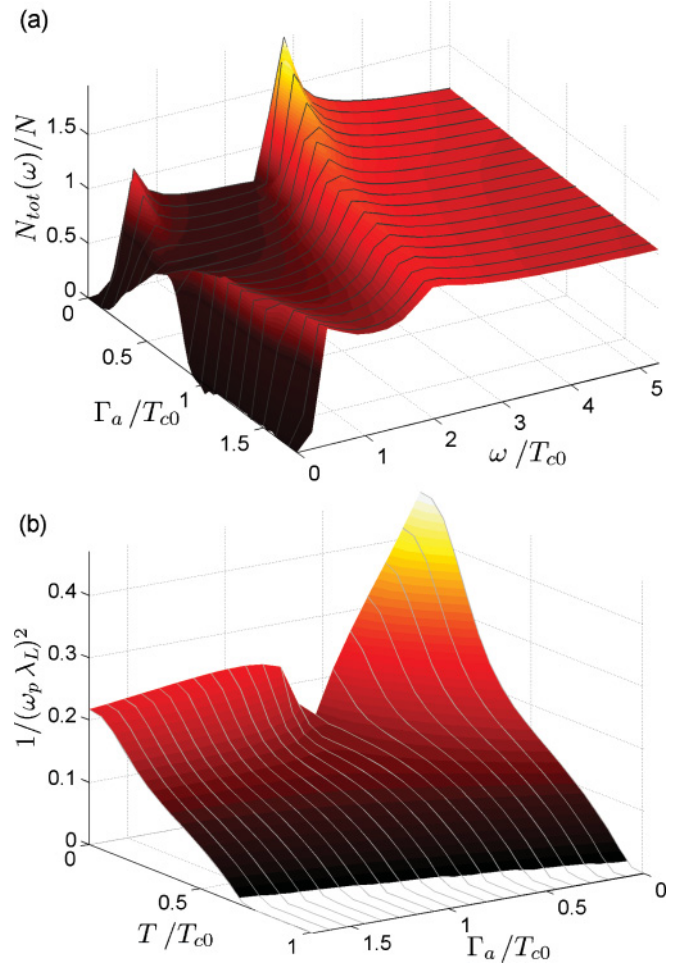

FIG. 3. (Color online) (a) Density of states $N_{\mathrm{tot}}(\omega)/N$ vs Γ_a/T_{c0} and ω/T_{c0} for $\langle \lambda \rangle > 0$ and impurity parameters $\tilde{\sigma} = 0.5$, $\eta = 1$, $N_b/N_a = 2$, $N = N_a + N_b$. (b) Total superfluid density $1/(\omega_p \lambda_L)^2$ vs Γ_a/T_{c0} and T/T_{c0}, where ω_p is the total plasma frequency and λ_L is the London penetration depth.

the lower gap is seen to close, leading to a finite residual $N_{\text{tot}}(\omega = 0)$, followed by a reopening of the gap. A similar behavior is reflected in the temperature dependence of the penetration depth [Fig. 3(b)], which varies in the clean limit with activated behavior controlled by the smaller gap, crossing over to T^2 in the gapless regime, to a new activated behavior in the s_{++} state in the dirty limit. Figure 3(b) should be compared to similar works, where the effect of scattering on the T-dependent superfluid density was calculated for a two-band s_{++} state.[13,22,23]

Conclusions. We have shown that in two-band models with an $s_{\pm}$ ground state, T_c has a universal dependence on the impurity scattering rate which can be calculated explicitly in terms of the interband to intraband impurity scattering rate ratio. We demonstrated that $s_{\pm}$ superconductivity may be quite robust against nonmagnetic impurities, depending on the ratio

of interband to intraband pairing coupling constants, and may even display a transition to an s_{++} gap structure with increasing disorder, which will manifest itself in thermodynamic and transport properties.

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