

Interplay of magnetic field and magnetic impurities in Ising superconductors

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Phonon-driven s -wave superconductivity is fundamentally antagonistic to uniform magnetism, and field-induced suppression of the critical temperature is one of its canonical signatures. Examples of the opposite are unique and require fortuitous cancellations and very fine parameter tuning. The recently discovered Ising superconductors violate this rule: an external magnetic field applied in a certain direction does not suppress superconductivity in an ideal, impurity-free material. We propose a simple and experimentally accessible system where the effects of spin-conserving and spin-flip scattering can be studied in a controlled way, namely NbSe₂ monolayers dozed with magnetic $3d$ atoms. We predict that the critical temperature is slightly increased by an in-plane magnetic field in NbSe₂ dozed with Cr. Due to the band spin splitting, magnetic spin-flip scattering requires a finite momentum transfer, while spin-conserving scattering does not. If the magnetic anisotropy is easy-axis, an in-plane field reorients the impurity spins and transforms spin-conserving scattering into spin-flip. The critical temperature is enhanced if the induced magnetization of NbSe₂ has a substantial long-range component, as is the case for Cr ions.

I. INTRODUCTION

It is well known that conventional superconductivity (excluding the Fulde-Ferrell-Larkin-Ovchinnikov spatially nonuniform superconductivity) cannot coexist with ferromagnetic order, but can, in principle, with ordered antiferromagnetism. This is usually rationalized in terms of superconducting coherence length being much larger than the lattice parameter, so that the staggered magnetization averages to zero over the corresponding length scale.

This rationalization, while appealing, is doubly incorrect. First, the cancellation of the staggered magnetization is not a sufficient condition: a recently discovered class of antiferromagnets [1, 2] is completely compensated by symmetry, yet features a finite exchange splitting incompatible with singlet superconductivity. Neither is it necessary: another recently discovered and hotly debated phenomenon, Ising superconductivity (IS), is, as we show in this paper, compatible with ferromagnetic order provided that the magnetization direction is perpendicular to the Ising vector and the exchange field H_{ex} is small compared to the spin-orbit coupling ξ_{SO} . The rationale here is that in this case the induced exchange splitting is quadratic in the exchange field as H_{ex}^2/ξ_{SO} , and even if the latter is much larger than the superconducting gap, $H_{ex} \gg \Delta$, the relevant parameter is still smaller: $H_{ex}^2/\xi_{SO} \ll \Delta$.

IS in two-dimensional materials is a rapidly growing field of theoretical and experimental research [3–10]. The combination of broken inversion symmetry and

strong spin-orbit coupling in monolayer transition metal dichalcogenides (TMD) leads to Fermi surfaces where the electron spin is perpendicular to the plane of the monolayer, and the spin direction flips between the Fermi sheets related to each other by time reversal. This has been experimentally confirmed by establishing, for example in NbSe₂, that the superconducting critical field is significantly higher when applied in-plane versus out-of-plane, and much larger than the Pauli limit [3].

Interaction of IS with impurities is highly nontrivial compared to the standard s -wave superconductors and has recently attracted considerable attention [6, 11, 12]. A particularly intriguing regime is magnetic impurities with sufficiently large characteristic scattering lengths and in-plane magnetization. This regime can be realized in a material close to ferromagnetism (superparamagnet) where a magnetic impurity generates a long-range ferromagnetic polarization. The scattering potential generated by such an impurity, in the momentum space, will be strong, but also strongly peaked at small momenta. As we discuss below, scattering momenta smaller than the spin-orbit splitting of the Fermi contours, $\Delta k_F = \xi_{SO}/v_F$, where ξ_{SO} is spin-orbit splitting, and v_F is the Fermi velocity, are not pair-breaking in the Abrikosov-Gor'kov regime [13]. On the contrary, randomly oriented impurities are liable to generate strong scattering at the wave vectors $q \sim 2\pi/d$, where d is the average distance between impurities.

This observation offers an intriguing opportunity: imagine an IS that hosts magnetic defects whose magnetic moment is out-of-plane in the ground state. If the

concentration of such defects is sufficiently small (the characteristic scale depends inversely on the scattering rate γ), the critical temperature T_c will exhibit the usual linear decline with increasing concentration, and superconductivity will disappear at the critical concentration $n_c \sim T_{c0}/\gamma$, where T_{c0} is the value of T_c in the clean material. Suppose the concentration is just above critical ($n \gtrsim n_c$), and the system is subjected to an in-plane external magnetic field H . The defect spins will then make an angle $\alpha = \cos^{-1}(HM/2\Delta E)$ with the plane, where M is the magnetic moment of the defect and ΔE the magnetic anisotropy energy (MAE) per spin. At the saturation field $H_s = 2\Delta E/M$ the spins complete their reorientation into the plane.

Suppose that the impurity-induced polarization $m(\mathbf{r})$ is slowly varying so that most of the spectral weight $\mu(\mathbf{q}) = \int d^2\mathbf{r} m(\mathbf{r}) \exp(i\mathbf{q}\mathbf{r})$ resides at $q \lesssim \Delta k_F$. Then the pair-breaking scattering rate will be reduced compared to the impurity spins oriented perpendicular to the plane. If the characteristic scale of the induced magnetization is larger than the inter-impurity distance, the effective magnetic scattering will be considerably reduced.

At this point, this becomes a game of numbers, a domain of computational materials science. Indeed, if the saturation field H_s is larger than the in-plane critical field H_{cx} , nothing interesting happens. However, if $H_s < H_{cx}$, then it may be possible that superconductivity at zero temperature, which is absent at zero field, will spontaneously appear at some $H_s < H < H_{cx}$. Examples of superconductivity triggered by magnetic field, especially of the conventional type, are extremely rare. A canonical example is the Jaccarino-Peter effect [14], which occurs through fine tuning of the external field to precisely compensate the existing ferromagnetic exchange field. Some heavy-fermion systems [15] feature *reentrant* (but not newly emerging) superconductivity, which is usually interpreted in terms of triplet pairing.

Magnetic field-triggered superconductivity in IS would, therefore, be rather unusual. By far, the best-studied IS is the NbSe₂ monolayer. The critical field there, while varying from sample to sample, can reach up to 40 T. This makes $H_s = H_{cx}$ at $\Delta E \sim 1.2$ meV/ μ_B , and the effect should be observable, say, for $\Delta E \lesssim 0.6$ meV/ μ_B at $H \approx H_{cx}/2$. Typically, MAE of 3d ions is smaller than that. Another piece of information is that bulk transition-metal diselenides, including NbSe₂, can be easily intercalated with 3d transition-metal atoms of Cr, Mn, Fe, and Co [16–18]. At sizable concentrations the latter order magnetically, forming interesting and non-trivial magnetic patterns. At small concentrations they behave, in the bulk, as magnetic pair breakers, as expected. Upon exfoliation, a lightly intercalated sample would create a monolayer dozed with magnetic ions. To our knowledge, so far this procedure has not been performed intentionally, and the superconducting properties of such dozed monolayers have not been studied.

In this paper we present a quantitative assessment of the possible response of the Ising superconductor NbSe₂

dozed with Cr, Mn, Fe, or Co to the in-plane magnetic field. Section II presents a general theory of magnetic pair-breaking in IS. Section III describes first-principles calculations of the magnetic moments and MAE for these ions, enabling the selection of a promising candidate system for the observation of field-induced superconductivity.

II. CRITICAL TEMPERATURE CALCULATION

Here we compute the critical temperature of IS in the presence of the long range magnetic impurities with a prescribed magnetization axis. The direct pair-breaking effect of the in-plane Zeeman field is negligible thanks to the protection due to Ising spin-orbit coupling (SOC), for $H \ll \xi_{SO}$. We also neglect the effect of scalar disorder which becomes pair-breaking at finite field. Indeed, for $H \ll \xi_{SO}$ the pair breaking scattering rate is small.

We consider two configurations, with impurities magnetized out-of-plane or in-plane. For short-range scattering, T_c is the same for both polarizations [19]. Here we specifically consider the situation when the typical range of impurity potential, ϱ , is comparable with or exceeds the length scale v_F/ξ_{SO} associated with SOC-induced splitting: $\varrho \gtrsim v_F/\xi_{SO}$. We extend the standard quasi-classical approach in order to describe this case.

We consider a magnetic atom such as Cr or Fe placed on top of a NbSe₂ monolayer, which is responsible for the magnetic scattering of the conduction electrons. Its magnetic moment \mathbf{M} induces spin-dependent potential both directly, through hybridization with the orbitals of the nearby host atoms and the resulting local interaction $J_L \mathbf{M} \boldsymbol{\sigma}$ of the Schrieffer-Wolff type, and indirectly, via the induced magnetization of the host atoms near the impurity. The latter adds an exchange term $-\sum_k J \boldsymbol{\mu}_k \boldsymbol{\sigma}$, where J is the Hund parameter and $\boldsymbol{\mu}_k$ are the magnetic moments of the host atoms k , which can be quite delocalized in space.

The input for the quasi-classical description are the scattering rates off the magnetic impurities. We write (half of) the rate of scattering on the i -th component of the magnetization as $\sigma_i(\mathbf{q}) = \zeta_i \mathcal{P}(\mathbf{q})$, where \mathbf{q} is the momentum transfer and $\mathcal{P}(0) \equiv 1$. The parameter ζ_i characterizes the overall strength of the scattering, and $\mathcal{P}(\mathbf{q})$ is a dimensionless form-factor reflecting the delocalized character of the induced magnetization in the host. According to Fermi's golden rule, for a random distribution of impurities,

$$\sigma_i(\mathbf{q}) = \pi n_m N_0 |J_L M_i - J \mu_i(\mathbf{q})|^2 \quad (1)$$

and $\zeta_i = \sigma_i(0)$, where n_m is the areal impurity density and N_0 is the density of host states at the Fermi level per spin. Because the orientation of the induced moments $\boldsymbol{\mu}_k$ relative to \mathbf{M} is determined by the sign of J_L , the two terms in the scattering amplitude typically add up. We will discuss the case of Cr/NbSe₂ in Sec. III.

Finally we specify the band structure model adequate for the present discussion. The Fermi surface of the TMD monolayer consists of the hole pockets centered at Γ as well as a pair of pockets at K and K' related to each other by time reversal. Although the effect of impurity spin reorientation is qualitatively similar for these two types of pockets, it is more pronounced for the pockets at K and K' . Indeed, SOC is nodeless at K and K' but has a node at Γ . The Fermi surface is connected at Γ and disconnected at K, K' . We will treat the two types of pockets separately. For conciseness, we present the basic steps of the calculation for the K (K') model in Sec. II A. Technical details of this calculation and a similar calculation for the Γ model are relegated to App. A and App. B, respectively.

A. The K (K') model

In this section we present the results for the critical temperature $T_c^{\perp,\parallel}$ for magnetic impurities polarized out-of-plane or in-plane for the K (K') model illustrated in Fig. 1. To highlight our results, in the present section we present the simplified isotropic version of the K (K') model, where we treat the two pockets as isotropic, neglecting trigonal warping. In particular, we regard N_0 as unaffected by SOC. Under these simplifying assumptions, we state the closed result for $T_c^{\parallel,\perp}$ formulated in a way that is similar to the Abrikosov-Gor'kov theory [13]. The details of the calculations for a more general anisotropic model are relegated to the App. A.

We disregard intervalley scattering for the following reasons. First, the states at K and K' have orthogonal orbital characters: $d_{xy} + id_{x^2-y^2}$ and $d_{xy} - id_{x^2-y^2}$, respectively. Therefore, scattering by a C_3 -symmetric impurity potential between the corresponding valleys is strongly suppressed [20]. Furthermore, even moderate intervalley scattering does not change the results qualitatively. Indeed, the key feature for the proposed effect is the absence of spin-flip scattering with small momentum transfer. This feature is unaffected by the inclusion of scattering to other distant regions in the Brillouin zone. This conclusion is confirmed by the calculation of the critical temperature for the Γ model in App. B.

Within the K (K') model, the electronic states at the Fermi level, $|\phi_{\mathbf{k}}, \eta, \beta\rangle$, are labeled by the valley η and spin β indices and the angle $\phi_{\mathbf{k}}$ formed by the momentum \mathbf{k} relative to the K (K') point with the unit vector \hat{x} . The valley index $\eta = \pm 1$ refers to K and K' pockets, and $\beta = \pm 1$ refers to the spin up and spin down polarization.

The valley-dependent Ising SOC has the following form: $\gamma_{\eta} = \eta\xi_{\text{SO}}$, which splits the originally spin-degenerate Fermi surface with the Fermi momentum k^F as shown in Fig. 1a. The Fermi momenta of the two spin polarized Fermi surfaces are $k_{\beta\eta}^F = k^F - \eta\beta\xi_{\text{SO}}/v_F$. Hence, in our notation, the electron in state $|\phi_{\mathbf{k}}, \eta, \beta\rangle$ has momentum $\mathbf{k} = k_{\beta\eta}^F \hat{\mathbf{k}}$ with $\hat{\mathbf{k}} \cdot \hat{x} = \cos \phi_{\mathbf{k}}$.

As discussed above, the scattering rate of an electron off the magnetic impurity from the initial state $|\phi_{\mathbf{k}}, \eta, \beta\rangle$ into the final state $|\phi_{\mathbf{k}'}, \eta', \beta'\rangle$ reads:

$$W_{\mathbf{k}\beta, \mathbf{k}'\beta'}^{\eta, \eta'} = \delta_{\eta, \eta'} \sum_{i=1}^3 \zeta_i \mathcal{P}(\mathbf{q}_{\beta\beta'}^{\eta, \eta'}) |\sigma_{\beta\beta'}^i|^2, \quad (2)$$

where, since the scattering occurs at the Fermi surface, $\mathbf{k} = k_{\beta\eta}^F \hat{\mathbf{k}}$, the scattering momentum $\mathbf{q}_{\beta\beta'}^{\eta, \eta'}$ depends on the valley and spin indices:

$$\mathbf{q}_{\beta\beta'}^{\eta, \eta'} = k_{\beta\eta}^F \hat{\mathbf{k}} - k_{\beta'\eta'}^F \hat{\mathbf{k}}'. \quad (3)$$

Let us introduce valley- and spin-dependent total scattering-out rates,

$$\Gamma_{\beta\beta'}^{\eta, \eta'} = \int_0^{2\pi} \frac{d\phi_{\mathbf{k}'}}{2\pi} W_{\mathbf{k}\beta, \mathbf{k}'\beta'}^{\eta, \eta'}. \quad (4)$$

The rates (4) are not independent. We have two independent spin-conserving scattering rates, $\Gamma_{\beta\beta} = \Gamma_{\beta\beta}^{\eta=1}$. The spin-conserving scattering rates for the other valley are related to $\Gamma_{\beta\beta}$ by time-reversal symmetry: $\Gamma_{\beta\beta}^{\eta} = \Gamma_{\bar{\beta}\bar{\beta}}^{\bar{\eta}}$, where we denote $\bar{\beta} = -\beta$, and $\bar{\eta} = -\eta$. All the spin-flip scattering rates are equal thanks to the detailed balance condition for intravalley scattering: $\Gamma_{\beta\bar{\beta}}^{\eta} = \Gamma_{\bar{\beta}\beta}^{\eta}$, combined with time-reversal symmetry. We denote the spin-flip scattering rate as Γ_f .

We express the pair-breaking effect for the out-of-plane or in-plane impurity polarization via the scattering rates introduced above:

$$\ln\left(\frac{T_{c0}}{T_c^{\perp}}\right) = \frac{1}{2} \sum_{\beta} \psi\left(\frac{1}{2} + \frac{\Gamma_{\beta\beta}}{\pi T_c^{\perp}}\right) - \psi\left(\frac{1}{2}\right), \quad (5a)$$

$$\ln\left(\frac{T_{c0}}{T_c^{\parallel}}\right) = \psi\left(\frac{1}{2} + \frac{\Gamma_f}{\pi T_c^{\parallel}}\right) - \psi\left(\frac{1}{2}\right). \quad (5b)$$

Here ψ is the digamma function. These results reflect the fact that the impurities polarized out-of-plane conserve, and in-plane flip, the electronic spin.

In a standard situation, without SOC and/or with a short-range scattering potential the pair breaking is isotropic, we have $\Gamma_f \approx \Gamma_{\beta\beta}$, and hence the spin orientation of impurities plays no role in the T_c suppression. In the present case, because of the SOC splitting, spin-flip scattering requires a finite momentum transfer, $|\mathbf{q}_{\beta\bar{\beta}}^{\eta}| \geq \xi_{\text{SO}}/v_F$. For the spin conserving transition, however, $|\mathbf{q}_{\beta\beta}^{\eta}| = k_{\beta\eta}^F [2(1 - \hat{\mathbf{k}} \cdot \hat{\mathbf{k}}')]^{1/2}$ can be arbitrarily small. Therefore, for $\varrho \gtrsim v_F/\xi_{\text{SO}}$, $\Gamma_{\beta\beta}^{\eta} \gg \Gamma_{\beta\bar{\beta}}^{\eta}$. This amounts to $\Gamma_{\beta} \gg \Gamma_f$ and to $T_c^{\parallel} > T_c^{\perp}$. As a result, field-induced superconductivity occurs at $T_c^{\perp} < T < T_c^{\parallel}$.

Note that Eq. (5a) contains an average of two digamma functions while usually, when more than one pair-breaking mechanisms are present, the pair-breaking parameters are instead added in the argument of a single

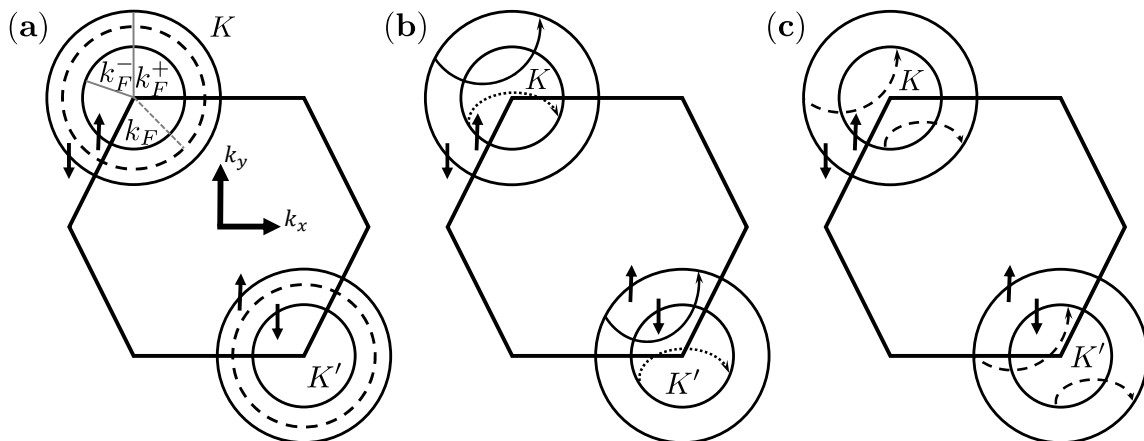


FIG. 1. In a $K(K')$ model the two hole pockets are centered at the two corners of the hexagonal Brillouin zone. (a) Fermi surface spin splitting due to the SOC. The original Fermi momentum k^F for the spin unpolarized Fermi surface turns to a two distinct Fermi momenta $k_F^\pm = k_F \pm \xi_{\text{SOC}}/v_F$. (b) Pair breaking processes active for magnetic impurities polarized out-of-plane. (c) The same as in (b) but for in-plane polarized impurities.

digamma function [21]. This difference is due to the special feature of the spin-conserving scattering, which occurs separately on two distinct spin-split Fermi surfaces. We also note that formally the above results are consistent with the results of Ref. [22]. The latter, however, cannot be applied as is because, if viewed as a two-band problem, each band contains electrons with a definite spin making up only “half” of a Cooper pairs.

III. FIRST-PRINCIPLES CALCULATIONS

Since no experimental data are available for transition-metal ions deposited on monolayer NbSe₂, we first gauge our methodology against intercalated bulk NbSe₂, where a limited amount of data is available. We consider a $3 \times 3 \times 1$ supercell constructed from the unit cell of bulk NbSe₂ ($a = 3.44 \text{ \AA}$, $c = 12.55 \text{ \AA}$) intercalated with one transition-metal (TM) atom (Cr, Mn, Fe, or Co) per supercell in its lowest energy position on top of a Nb atom [23]. The impurity concentration is thus 1.8%. The structure is optimized using the projector-augmented wave (PAW) method [24] implemented in the Vienna *Ab Initio* Simulation Package (VASP) [25, 26]. The generalized gradient approximation of Perdew-Burke-Ernzerhof (PBE) [27] is used as the exchange-correlation functional. The atomic positions are relaxed using a $3 \times 3 \times 2$ Γ -centered k -point grid until the forces on all atoms are less than 0.01 eV/\AA . The monolayer structures are obtained by removing one of the NbSe₂ layers from the bulk structure and relaxed using the same criterion.

To speed up the calculations, the electronic structure and MAE of the resulting structures was studied using the OpenMX code utilizing a pseudo-atomic orbital basis set [28, 29]. The charge and spin densities were obtained from a self-consistent calculation with-

out SOC and kept fixed in the subsequent MAE calculations. MAE is determined as the difference in band energies calculated with the magnetization aligned in-plane and out-of-plane. Positive MAE corresponds to easy-axis anisotropy. We have compared our results using OpenMX without LDA+U in monolayer NbSe₂ doped with different impurities with the results using VASP. The agreement is excellent for Co and Mn. For Cr and Fe, the agreement is good for MAE but OpenMX gives 15% larger magnetic moments.

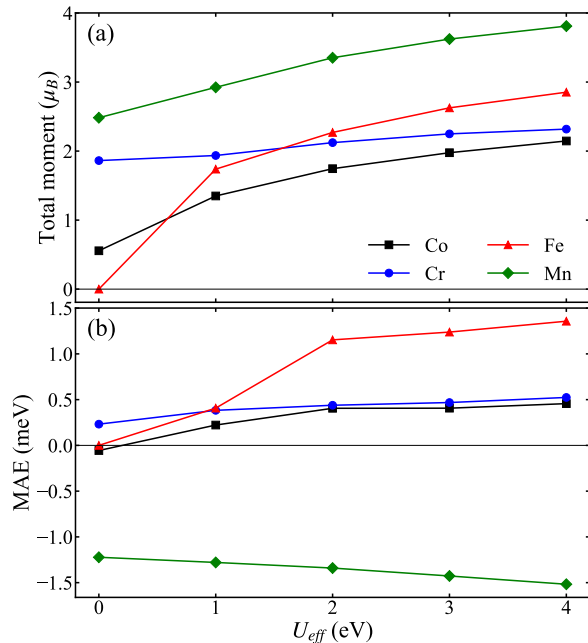


FIG. 2. Dependence of magnetic moments and MAEs on U_{eff} for bulk NbSe₂ intercalated with Cr, Mn, Fe, or Co.

We use the LDA+U method [30] to better account for the correlation effects on the $3d$ ions. Figure 2 shows the total magnetic moments and MAE for bulk NbSe₂ intercalated with different impurities as a function of $U_{\text{eff}} = U - J$, where U and J are the on-site Coulomb and exchange parameters. The magnetic moments monotonically increase with U_{eff} . Note that Fe-intercalated NbSe₂ is magnetic only if a small but finite U_{eff} is included.

The effective magnetic moments for Co_{0.012}NbSe₂, Mn_{0.0012}NbSe₂, and Fe_xNbSe₂ were reported at 0.6, 4.2, and 3.2 μ_B , respectively [17, 18]. Reasonable agreement with these data for Mn and Fe can be obtained with $U_{\text{eff}} = 4$ eV, while for Co the best agreement is obtained without LDA+U. This is in line with the general expectation that Co is the least, and Mn the most, correlated of the three ions. MAE also depends monotonically on U and retains the same sign for all intercalants except Co, where it changes sign at a small value of U_{eff} . Because the results for Cr (where no experimental data are available) depend little on U_{eff} , we set $U_{\text{eff}} = 0$ for Cr in the following.

Having determined the optimal U_{eff} from the bulk calculations, we evaluate the MAE, the total magnetic moments, and spin-flip fields for monolayer NbSe₂ doped with different impurities. The results are listed in Table I. Here Co, Cr, and Fe have larger magnetic moments compared to the intercalated bulk, and they all have positive MAE with a spin-flip field that is less than 30 T. For Co, the magnetic moment is close to the low-spin $3d^7$ -electron configuration of Co²⁺ ($S = 1/2$). For Mn, it is close to the $3d^4$ configuration of Mn³⁺ ($S = 2$). Cr and Fe are potentially suitable candidates as they have experimentally accessible spin-flip fields.

Impurity	U_{eff} eV	MAE ΔE meV	Total moment μ_B	TM moment μ_B	H_s T
Co	0	1.30	1.57	1.83	28
Cr	0	1.44	3.58	4.31	14
Fe	4	1.04	3.47	3.59	10
Mn	4	-0.67	4.56	4.89	—

TABLE I. Calculated MAE, total magnetic moments, TM magnetic moments, and in-plane saturation fields in monolayer NbSe₂ doped with magnetic atoms.

We now examine the distribution of the induced magnetic moments on the Nb atoms in Fe/NbSe₂ and Cr/NbSe₂ systems. As shown in Ref. [23], the exchange coupling between TM adatoms on NbSe₂ is rather long-ranged. Therefore, we use a 15×15 supercell to minimize interaction between the impurities, although even at this large size the results may not be fully converged. We also note that the use of the PBE exchange-correlation potential results in a longitudinal remnant of the spin density wave (SDW) in NbSe₂; we suppress it by using the local density approximation (LDA) in this calculation (with U_{eff} included for Fe), which is performed in VASP.

Figure 3 shows the total magnetic moment induced on Nb atoms within a circle of radius r from the one di-

rectly underneath the impurity. In Fe/NbSe₂ there is a strong cancellation between positive and negative spin moments, and, as a result, the Fourier transform $\mu(\mathbf{q})$ is expected to peak at finite \mathbf{q} . In contrast, in Cr/NbSe₂ the induced magnetization is accumulated, almost monotonically, over several coordination spheres. This behavior produces $\mu(\mathbf{q})$ that is peaked at $\mathbf{q} = 0$, which is favorable for field-induced superconductivity. The difference between Fe and Cr is likely due to the different hybridization patterns. In the following we focus on the Cr/NbSe₂ system.

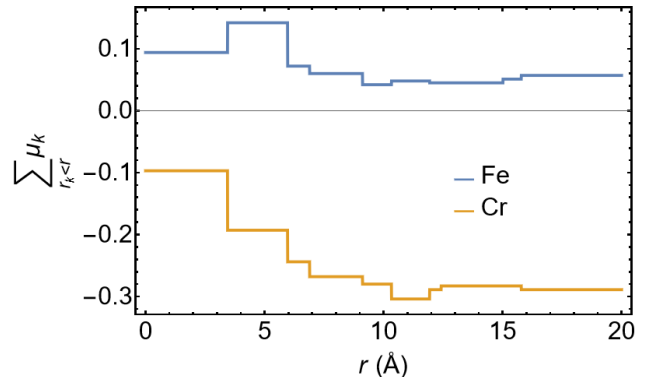


FIG. 3. Total spin moment induced on Nb atoms in Fe/NbSe₂ and Cr/NbSe₂ within a circle of radius r centered at the Nb atom directly underneath the impurity.

According to Eq. (1), the scattering amplitude has contributions from local interaction with the impurity and from the delocalized interaction with the spin moments induced on the Nb atoms. The relative magnitude of these two terms can be estimated from their contributions to the exchange splitting Δ near the Fermi level in the 15×15 supercell. The total magnetic moment of this supercell is 3.54 μ_B , which includes 5 μ_B contributed by the five filled majority-spin bands deriving from the deep $3d$ states of Cr. The remaining $-1.46 \mu_B$ reflect the magnetization of the native bands of NbSe₂. It includes the magnetization induced on Nb ions as well as an admixture of the minority-spin Cr orbitals. Δ can be found by dividing this number by the DOS N_0 per spin in the up-doped layer ($1.35 \text{ eV}^{-1}/\text{f.u.}$), which gives $\Delta = 4.8 \text{ meV}$. Direct matching of the majority- and minority-spin DOS near the Fermi level suggests a somewhat smaller $\Delta \approx 4 \text{ meV}$.

On the other hand, the contribution of the induced Nb moments to Δ in the 15×15 supercell can be estimated as $J\mu_{\text{tot}}/15^2 \approx 0.8 \text{ meV}$, where $J \approx 0.6 \text{ eV}$ and $\mu_{\text{tot}} = -0.29 \mu_B$ is the total spin moment induced on the Nb atoms. Thus, we estimate that Hund exchange with the induced moments on the Nb atoms contributes about 20% to the total scattering amplitude near the Fermi level, and hence $J\mu(0) \approx -0.2J_L M$. (Note that $J_L < 0$ in Cr/NbSe₂.) The scattering form-factor $\mathcal{P}(\mathbf{q})$ for Cr/NbSe₂ is then obtained from Eq. (1) and shown in Fig. 4.

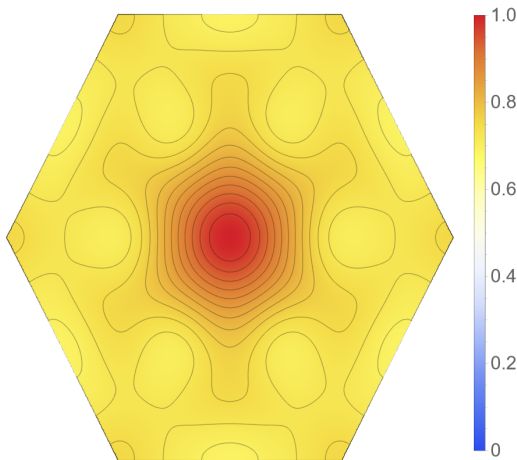


FIG. 4. Scattering form-factor $\mathcal{P}(\mathbf{q})$ for Cr/NbSe₂ plotted in the first Brillouin zone. Contours are drawn between 0.7 and 0.975 in intervals of 0.025.

IV. THE EFFECT OF SPIN REORIENTATION

In this section we estimate the suppression of T_c in NbSe₂ doped with magnetic ions which occurs due to the magnetization induced in NbSe₂. As discussed in section II, the crucial information is contained in the Fourier transform of the induced magnetization, $\mu(\mathbf{q})$.

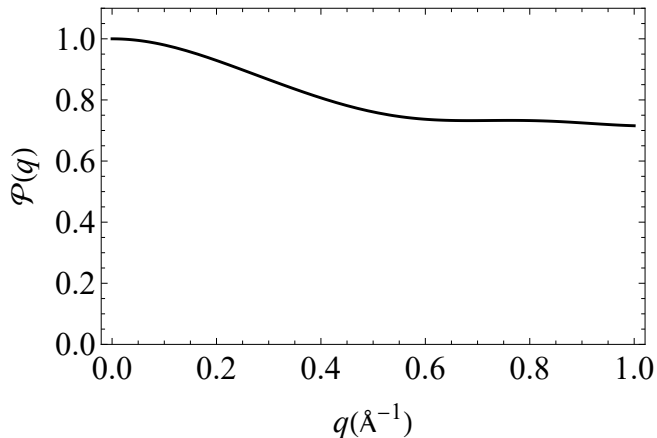


FIG. 5. Isotropic approximation for the form-factor $\mathcal{P}(q)$ in Cr/NbSe₂ obtained by averaging $\mathcal{P}(\mathbf{q})$ shown in Fig. 4 over the azimuthal angle. This approximation is applied and shown here for $q < G/2$ where $G = 4\pi/(\sqrt{3}a) \approx 2 \text{ \AA}^{-1}$ is the length of the shortest reciprocal lattice vector.

We have computed the critical temperature for the $K(K')$ model for out- and in-plane orientation of impurities. The calculation was performed using the isotropic approximation of the form-factor shown in Fig. 5. This approximation is sufficient because the actual momentum transfer does not exceed twice the Fermi momentum of the electronic pockets, which is about $0.7 \text{ \AA}^{-1} < G/2$. Trigonal warping can be neglected for such momenta. We

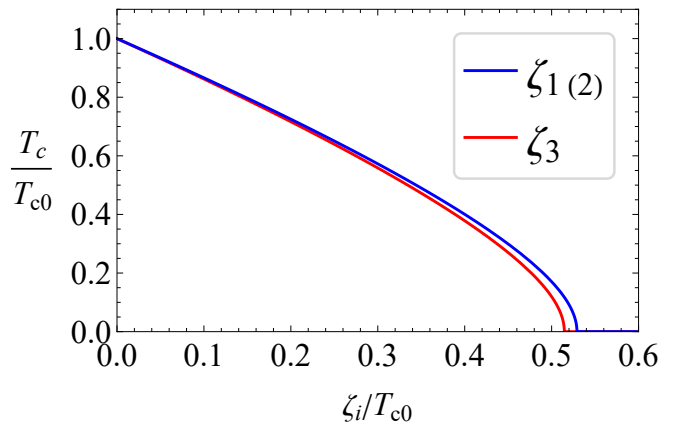


FIG. 6. The critical temperature T_c as function of ζ_i with the magnetic impurities in-plane (blue line) and out-of-plane (red line), calculated by solve Eqs. (5b) and (5a) respectively. The form factor is shown in Fig. 5 and the parameters are $2mE_F/\hbar^2 = 0.075 \text{ \AA}^{-2}$, $\xi_{\text{SO}}/E_F = 0.5$. T_{c0} is the critical temperature without magnetic impurities

have checked that this approximation produces a negligible error in the calculations of T_c . The results are contained in Eqs. (5) and are presented in Fig. 6.

The magnitude of the effect, namely the difference between the values of T_c for two spin orientations, follows from the magnetic interaction rather localized in space. The source of this localization is the direct interaction with the magnetic ion. We have checked that the effect is much stronger if the magnetic form-factor is less localized (see App. A, and Fig. 7). In addition, the increase in T_c caused by the magnetic field occurs also in the Γ -model of the electronic dispersion. The results for the Γ -model are presented in Fig. 8 of App. B.

We can estimate the impurity concentration needed to achieve field-induced superconductivity as follows. For the exchange splitting $\Delta = 4.8 \text{ meV}$ we find, using Eq. (1), that the critical temperature 4 K of a clean system is suppressed to zero at the impurity concentration of $1.4 \times 10^{10} \text{ cm}^{-2}$. At this concentration the typical distance between the impurity atoms is on the order of 100 nm, and our analysis assuming isolated impurities is well justified.

V. CONCLUSIONS

We predicted a novel effect presenting another manifestation of the unique nature of Ising superconductivity: a parametric regime where superconductivity is strictly absent at zero field in the presence of dilute, easy-axis magnetic impurities but can be “turned on” by a moderate in-plane magnetic field. Such “incipient” superconductivity, which requires a magnetic field to reveal itself, is unique and counterintuitive.

We presented a microscopic theory and quantitative DFT calculation of this effect, demonstrating that mono-

layer NbSe₂ lightly doped with Cr atoms is a promising material platform for its observation. Since Cr can be easily intercalated into bulk NbSe₂, experimental verification of our prediction should be feasible.

The physical meaning of the effect of field-induced superconductivity is quite transparent and is similar to the famous ‘‘Ising protection’’ against the uniform in-plane magnetic field. Indeed, in the limit of a dominant forward scattering, that is, a small q scattering, the pair-breaking effect of impurities is analogous to the pair-breaking effect of Zeeman splitting (in a way, a uniform magnetic field can be thought of as a giant impurity with scattering limited to $q = 0$). ‘‘Small’’ here means smaller than ξ_{SO}/v_F . In NbSe₂ the effect is relatively weak, albeit expected to be detectable, because of the proximity to a spin density wave at $\mathbf{Q} \approx (0.2, 0, 0)$ [31, 32], which transfers some weight for small q to $q \sim Q$. On the other hand, NbSe₂ is also close to a ferromagnetic ($q = 0$) instability[31, 33], albeit not as close as to the SDW. Potentially, an Ising superconductor that retains proximity to a ferromagnetic instability, but not to an SDW, would be an even better candidate to discover this effect.

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Appendix A: Details of the calculation of the critical temperature for the $K(K')$ model

Here we present a more detailed derivation of the results, (5). We start with the model Hamiltonian presented as a sum

$$H = H_0 + H_{SOC} + H_p + H_{dis}^s + H_{dis}^m. \quad (A1)$$

In Eq. (A1), $H_0 = \sum_{\mathbf{k}, \eta, \beta} \xi_{\mathbf{k}} a_{\eta\mathbf{k}\beta}^\dagger a_{\eta\mathbf{k}\beta}$, where $a_{\eta\mathbf{k}\beta}^\dagger$ is the operator creating an electron in the state, $|\phi_{\mathbf{k}}, \eta, \beta\rangle$, and $\xi_{\mathbf{k}}$ is the kinetic energy counted from the Fermi energy, E_F . The SOC Hamiltonian reads,

$$H_{SOC} = \sum_{\eta} \sum_{\mathbf{k}, \beta, \beta'} \boldsymbol{\gamma}_{\eta} \cdot \boldsymbol{\sigma}_{\beta\beta'} a_{\eta\mathbf{k}\beta}^\dagger a_{\eta\mathbf{k}\beta'} \quad (A2)$$

where the Ising SOC polarizes spin out-of-plane, $\boldsymbol{\gamma}_{\eta} = \hat{z}\gamma_{\eta}$. We assume the pairing interaction to be active in a

spin singlet channel,

$$H_p = \frac{1}{2} \sum_{\eta, \eta'} \sum_{\beta_{1,2}, \beta'_{1,2}} \sum_{\mathbf{k}, \mathbf{k}'} v_K [i\sigma_y]_{\beta_1\beta_2} [i\sigma_y]_{\beta'_1\beta'_2}^* \times a_{\eta\mathbf{k}\beta_1}^\dagger a_{\eta\mathbf{k}\beta_2}^\dagger a_{\eta'\mathbf{k}'\beta'_2} a_{\eta'\mathbf{k}'\beta'_1}. \quad (A3)$$

Scalar disorder represented by the H_{dis}^s term is inconsequential as expected from the Anderson theorem, and the interaction of electrons with the magnetic impurities placed at random locations \mathbf{R}_i is contained in the exchange coupling:

$$H_{dis}^m = \sum_{\mathbf{R}_i, \mathbf{k}, \mathbf{k}'} e^{i\mathbf{R}_i(\mathbf{k}-\mathbf{k}')} \sum_{\eta\beta, \eta'\beta'} [J\boldsymbol{\mu}(\mathbf{k}-\mathbf{k}') + J_L\mathbf{M}] \cdot \boldsymbol{\sigma}_{\beta\beta'} \times a_{\eta\mathbf{k}\beta}^\dagger a_{\eta\mathbf{k}'\beta'}. \quad (A4)$$

The crucial feature of Eq. (A4) is that for $\mathbf{M} \parallel \hat{z}$ (and hence $\boldsymbol{\mu} \parallel \hat{z}$) the transitions caused by H_{dis}^m are spin-conserving, while for $\mathbf{M} \perp \hat{z}$ (and $\boldsymbol{\mu} \perp \hat{z}$) they are spin-flipping. Equation (A4) gives rise to the scattering rate stated in Eq. (2).

We have approached the current problem by extension of the quasi-classical formalism used by two of us previously to study the magnetic disorder [19]. In the case of the $K(K')$ -model we extend the usual four-dimensional space including the particle-hole (Nambu) and spin degrees of freedom to the eight dimensional space which includes in addition, the valley degree of freedom. We denote the three sets of Pauli matrices $\boldsymbol{\rho}$, $\boldsymbol{\sigma}$ and $\boldsymbol{\tau}$ operate in Nambu, spin and valley spaces, respectively. We also denote by ρ_0 , σ_0 and τ_0 the unit matrices operating in these spaces. A quantity, \mathcal{O} defined in this extended eight dimensional space is denoted by the check sign, $\check{\mathcal{O}}$. The basic object is the Green function defined as follows,

$$\check{G}(\eta\mathbf{k}, \omega_n) = \begin{bmatrix} \hat{G}^{\eta\eta}(\mathbf{k}, \omega_n) & \hat{G}^{\eta\bar{\eta}}(\mathbf{k}, \omega_n) \\ \hat{G}^{\bar{\eta}\eta}(\mathbf{k}, \omega_n) & \hat{G}^{\bar{\eta}\bar{\eta}}(\mathbf{k}, \omega_n) \end{bmatrix}, \quad (A5)$$

where $\omega_n = (2n + 1)\pi T$ are the Matsubara frequencies with integer n , and the four by four Green functions have a form,

$$\hat{G}^{\eta\eta'} = \begin{bmatrix} G^{\eta\eta'}(\mathbf{k}, \omega_n) & F^{\eta\eta'}(\mathbf{k}, \omega_n) \\ -[F^{\eta\eta'}(-\mathbf{k}, \omega_n)]^* & -[G^{\eta\eta'}(-\mathbf{k}, \omega_n)]^* \end{bmatrix}, \quad (A6)$$

with each entry being a two by two matrix in spin space,

$$G_{\beta\beta'}^{\eta\eta'}(\mathbf{k}, \omega_n) = - \int_0^{T^{-1}} d\tau e^{i\omega_n\tau} \langle T_{\tau} a_{\mathbf{k}\eta\beta}(\tau) a_{\mathbf{k}\eta'\beta'}^\dagger \rangle, \quad (A7)$$

where $a_{\eta\mathbf{k}\beta}(\tau) = e^{\tau H} a_{\eta\mathbf{k}\beta} e^{-\tau H}$. Within the mean field approach, the Green function, Eq. (A5) satisfies the Gor'kov equation,

$$[i\omega_n \check{\mathbb{1}} - \check{H}_{\text{BdG}} - \check{\Sigma}] \check{G} = \check{\mathbb{1}}, \quad (A8)$$

where $\hat{\mathbb{1}} = \rho_0 \sigma_0 \tau_0$. The Bogoliubov-de-Gennes (BdG) Hamiltonian takes the form

$$\check{H}_{\text{BdG}} = \begin{bmatrix} \xi_k + \gamma_\eta \cdot \boldsymbol{\sigma} & 0 & 0 & \underline{\Delta} \\ 0 & -\xi_k - \gamma_\eta \cdot \boldsymbol{\sigma}^T & \underline{\Delta}^\dagger & 0 \\ 0 & \underline{\Delta} & \xi_k + \gamma_{\bar{\eta}} \cdot \boldsymbol{\sigma} & 0 \\ \underline{\Delta}^\dagger & 0 & 0 & -\xi_k - \gamma_{\bar{\eta}} \cdot \boldsymbol{\sigma}^T \end{bmatrix} \quad (\text{A9})$$

where for shortness we write $\xi_k \sigma_0$ as ξ_k , and the OP is a singlet, $\underline{\Delta} = \psi_0 i \sigma_2$.

The self-energy $\check{\Sigma}$ in the Gor'kov equation, (A8) incorporates the effects of scattering on the magnetic impurities:

$$\check{\Sigma}(\eta \mathbf{k}, \omega_n) = N_0^{-1} \pi^{-1} \sum_{i=1}^3 \zeta_i \int \frac{d^2 \mathbf{k}'}{(2\pi)^2} \mathcal{P}(\mathbf{k} - \mathbf{k}') \times \check{V}_i \check{G}(\eta \mathbf{k}', \omega_n) \check{V}_i, \quad (\text{A10})$$

where $\check{V}_1 = \rho_3 \sigma_1 \tau_0$, $\check{V}_2 = \rho_0 \sigma_2 \tau_0$, and $\check{V}_3 = \rho_2 \sigma_3 \tau_0$ describes the structure of the disorder scattering matrix elements due to the i -th component of the impurity spin polarization. In Eq. (A10) and throughout the paper we have neglected the scattering between the K and K' pockets.

The form of the BdG Hamiltonian, (A9) suggests that the dimension of the Hilbert space can be reduced. Indeed, we show that it can be reduced to two decoupled problems in the four-dimensional space that is a product of the particle-hole and spin spaces. The above reduction can in principle be made impossible because of the self energy, (A10). Yet, one can readily check by way of iterations that with this self-energy the blocks of Eq. (A6) satisfy, $G^{\eta\bar{\eta}} = 0$ and $F^{\eta\eta} = 0$. The matrix blocks, \hat{G} take the form,

$$\hat{G}^{\eta\eta} = \begin{bmatrix} G^{\eta\eta}(\mathbf{k}, \omega_n) & 0 \\ 0 & -[G^{\eta\eta}(-\mathbf{k}, \omega_n)]^* \end{bmatrix}, \quad (\text{A11a})$$

$$\hat{G}^{\eta\bar{\eta}} = \begin{bmatrix} 0 & F^{\eta\bar{\eta}}(\mathbf{k}, \omega_n) \\ -[F^{\eta\bar{\eta}}(-\mathbf{k}, \omega_n)]^* & 0 \end{bmatrix}. \quad (\text{A11b})$$

Equation (A11) shows that we can limit the consideration to the four dimensional BdG Hamiltonian comprized of the (1, 1), (1, 4), (4, 1) and (4, 4) two by two blocks of the original BdG Hamiltonian, (A9),

$$\hat{H}_{\text{BdG}} = \begin{bmatrix} \xi_k + \gamma_\eta \cdot \boldsymbol{\sigma} & \underline{\Delta} \\ \underline{\Delta}^\dagger & -\xi_k - \gamma_{\bar{\eta}} \cdot \boldsymbol{\sigma}^T \end{bmatrix} \quad (\text{A12})$$

The same blocks of the Green function, (A5) according to Eq. (A6) comprize the reduced Green function,

$$\hat{G}(\mathbf{k}\eta, \omega_n) = \begin{bmatrix} G^{\eta\eta}(\mathbf{k}, \omega_n) & F^{\eta\bar{\eta}}(\mathbf{k}, \omega_n) \\ -F^{\eta\bar{\eta}*}(-\mathbf{k}, \omega_n) & -G^{\eta\eta}(-\mathbf{k}, \omega_n) \end{bmatrix} \quad (\text{A13})$$

which has a standard form with the added information that the normal state Hamiltonian is diagonal in the valley index, while the pairing term of the Hamiltonian is off diagonal. The four dimensional equivalent of Eq. (A8),

$$\left[i\omega_n \hat{\mathbb{1}} - \hat{H}_{\text{BdG}} - \hat{\Sigma} \right] \hat{G} = \hat{\mathbb{1}}, \quad (\text{A14})$$

where $\hat{\mathbb{1}} = \rho_0 \sigma_0$.

As is the case of the Abrikosov-Gor'kov problem, the further reduction of (A13) down to the particle-hole space is possible. Specifically, we have two coupled problems defined for the inner and outer blocks of Eq. (A13) and labeled by the spin-index, $\beta = \pm 1$,

$$\bar{G}^{(\beta)}(\eta \mathbf{k}, \omega_n) = \begin{bmatrix} G_{\beta\beta}^{\eta\eta}(\mathbf{k}, \omega_n) & F_{\beta\beta}^{\eta\bar{\eta}}(\mathbf{k}, \omega_n) \\ -F_{\beta\beta}^{\eta\eta*}(-\mathbf{k}, \omega_n) & -G_{\beta\beta}^{\eta\bar{\eta}*}(-\mathbf{k}, \omega_n) \end{bmatrix} \quad (\text{A15})$$

Let us introduce the standard definition of the quasi-classical Green function,

$$\bar{g}^{(\beta)}(\eta \hat{\mathbf{k}}, \omega_n) = \int \frac{d\xi_k}{\pi} i \rho_3 \bar{G}^{(\beta)}(\eta \mathbf{k}, \omega_n). \quad (\text{A16})$$

The quasi-classical Green function satisfies the Eilenberger equation,

$$\left[\left(i\omega_n \rho_0 - \bar{S}_\eta^{(\beta)} - \bar{\Sigma}^{(\beta)}(\eta \hat{\mathbf{k}}, \omega_n) \right) \rho_3, \bar{g}^{(\beta)}(\eta \hat{\mathbf{k}}, \omega_n) \right] = 0 \quad (\text{A17})$$

where

$$\bar{S}_\eta^{(\beta)} = \beta \begin{pmatrix} \gamma_\eta & \psi_0 \\ \psi_0^* & -\gamma_\eta \end{pmatrix}, \quad (\text{A18})$$

and the self-energy follows from Eq. (A10) by reducing it to the two-by-two matrix in the same way as we did it for the Green function. Namely, for the contribution to the self energy from the j th component of the magnetization we have for the in-plane polarized impurities, $j = 1, 2$

$$\bar{\Sigma}_j^{(\beta)} = -i \zeta_j \rho_0 \left\langle \bar{g}^{(\beta)}(\eta \hat{\mathbf{k}}', \omega_n) \mathcal{P}(\mathbf{q}_{\beta\beta}^\eta) \right\rangle_{\hat{\mathbf{k}}'} \rho_3, \quad (\text{A19})$$

and for the impurities polarized out-of-plane we get

$$\bar{\Sigma}_3^{(\beta)} = -i \zeta_3 \rho_3 \left\langle \bar{g}^{(\beta)}(\eta \hat{\mathbf{k}}', \omega_n) \mathcal{P}(\mathbf{q}_{\beta\beta}^\eta) \right\rangle_{\hat{\mathbf{k}}'} \rho_0. \quad (\text{A20})$$

As explained above the self-energies, (A19) and (A20) describe spin flipping and spin conserving scattering, respectively.

To solve Eq. (A17) we use the following parametrization of the quasi-classical Green function,

$$\bar{g}^{(\beta)}(\eta \hat{\mathbf{k}}, \omega_n) = i g_0^{(\beta)}(\eta \hat{\mathbf{k}}, \omega_n) \rho_0 + g_3^{(\beta)}(\eta \hat{\mathbf{k}}, \omega_n) \rho_3 + i f_1^{(\beta)}(\eta \hat{\mathbf{k}}, \omega_n) \rho_1 + i f_2^{(\beta)}(\eta \hat{\mathbf{k}}, \omega_n) \rho_2. \quad (\text{A21})$$

The functions introduced in Eq. (A21) satisfy the relations,

$$\begin{aligned} [g_{0,3}^{(\beta)}(\eta(-\hat{\mathbf{k}}), \omega_n)]^* &= g_{0,3}^{(\bar{\beta})}(\eta\hat{\mathbf{k}}, \omega_n), \\ [f_{1,2}^{(\beta)}(\eta(-\hat{\mathbf{k}}), \omega_n)]^* &= f_{1,2}^{(\bar{\beta})}(\eta\hat{\mathbf{k}}, \omega_n). \end{aligned} \quad (\text{A22})$$

For our purposes it is sufficient to find the functions, $f_{1,2}$ to the linear order in OP. The linearization of the Eilenberger equation, (A17) results in the following equations, omitting the Matsubara frequency argument for shortness,

$$\begin{aligned} &\zeta_3 \left\langle \left(f_1^{(\beta)}(\eta\hat{\mathbf{k}}') + f_1^{(\beta)}(\eta\hat{\mathbf{k}}) \right) \mathcal{P}(\mathbf{q}_{\beta\bar{\beta}}^\eta) \right\rangle_{\hat{\mathbf{k}}'} \\ &- (\zeta_1 + \zeta_2) \left\langle \left(f_1^{(\bar{\beta})}(\eta\hat{\mathbf{k}}') - f_1^{(\bar{\beta})}(\eta\hat{\mathbf{k}}) \right) \mathcal{P}(\mathbf{q}_{\beta\bar{\beta}}^\eta) \right\rangle_{\hat{\mathbf{k}}'} \\ &= -|\omega_n| f_1^{(\beta)}(\eta\hat{\mathbf{k}}), \end{aligned} \quad (\text{A23a})$$

$$\begin{aligned} &\zeta_3 \left\langle \left(f_2^{(\beta)}(\eta\hat{\mathbf{k}}') + f_2^{(\beta)}(\eta\hat{\mathbf{k}}) \right) \mathcal{P}(\mathbf{q}_{\beta\bar{\beta}}^\eta) \right\rangle_{\hat{\mathbf{k}}'} \\ &- (\zeta_1 + \zeta_2) \left\langle \left(f_2^{(\bar{\beta})}(\eta\hat{\mathbf{k}}') - f_2^{(\bar{\beta})}(\eta\hat{\mathbf{k}}) \right) \mathcal{P}(\mathbf{q}_{\beta\bar{\beta}}^\eta) \right\rangle_{\hat{\mathbf{k}}'} \\ &= -|\omega_n| f_2^{(\beta)}(\eta\hat{\mathbf{k}}) - \beta i \psi_0. \end{aligned} \quad (\text{A23b})$$

Equation (A23a) yields $f_1^{(\beta)}(\eta\hat{\mathbf{k}}, \omega_n) = 0$. Equation (A23b) is easily solved in the case of the isotropic pockets and isotropic scattering assumed here. Thanks to the isotropy assumption, the functions $f_2^{(\beta)}(\eta\hat{\mathbf{k}}, \omega_n)$ are independent of the momentum direction, $\hat{\mathbf{k}}$. Hence Eq. (A23b) becomes an algebraic equation.

We consider separately the case of out- and in-plane polarized magnetic impurities. In the case of out-of-plane impurities $\zeta_{1,2} = 0$, and Eq. (A23b) gives,

$$f_{2,\perp}^{(\beta)}(\eta) = -\frac{i\beta\psi_0}{2\Gamma_{\beta\bar{\beta}}^\eta + |\omega_n|}, \quad (\text{A24})$$

and for the in-plane impurities

$$f_{2,\parallel}^{(\beta)}(\eta) = -\frac{i\beta\psi_0}{2\Gamma_{\beta\bar{\beta}}^\eta + |\omega_n|}. \quad (\text{A25})$$

These results has to be substituted into a linearized self-consistency conditions,

$$\pi T \sum_{\omega_n, \eta} \left[\frac{\psi_0}{|\omega_n|} - \frac{i}{2} \sum_{\beta} \beta f_{2\perp, \parallel}^{(\beta)}(\eta) \right] = 2\psi_0 \ln \left(\frac{T_{c0}}{T_{c\perp, \parallel}} \right), \quad (\text{A26})$$

The scattering rates are quadratic in the magnetization, in result, the time reversal symmetry implies $\Gamma_{\beta\bar{\beta}'}^\eta = \Gamma_{\bar{\beta}\beta'}^\eta$. We also have a detailed balance condition, $\Gamma_{\beta\bar{\beta}'}^\eta = \Gamma_{\bar{\beta}'\beta}^\eta$. As a result we can eliminate the summation over the valley index in Eq. (A26),

$$\pi T \sum_{\omega_n} \left[\frac{\psi_0}{|\omega_n|} - \frac{i}{2} \sum_{\beta} \beta f_{2\perp, \parallel}^{(\beta)}(\eta = 1) \right] = \psi_0 \ln \left(\frac{T_{c0}}{T_{c\perp, \parallel}} \right), \quad (\text{A27})$$

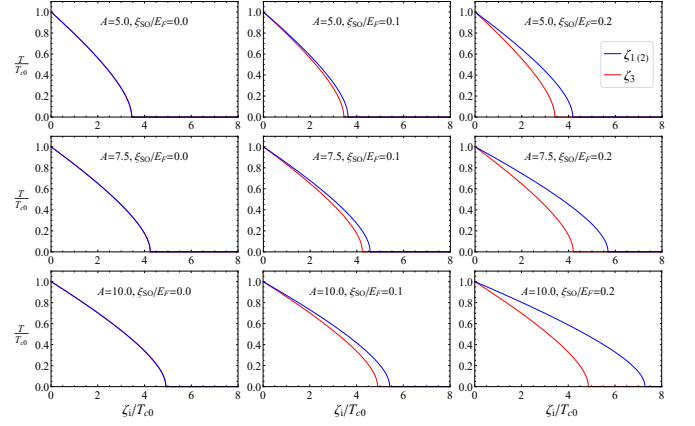


FIG. 7. Calculated T_c as a function of the parameters, ζ_i , $i = 1, 2, 3$ proportional to the impurity concentration for the $K(K')$ model. In the calculation, only one of ζ_i is non-zero. For the blue lines $\zeta_{1(2)} \neq 0$ and we solve Eq. (5b). For the red lines $\zeta_3 \neq 0$ and we solve Eq. (5a). Both axes are plotted in units of T_{c0} . Along the rows the parameter ξ_{SO}/E_F increases. Along the columns the parameter $A = \varrho^2 m E_F / \hbar^2$ increases. Here we take an isotropic Gaussian model for the form factor $\mathcal{P}(\mathbf{q}) = \exp[-(\varrho\mathbf{q})^2/2]$.

Substituting Eqs. (A24) and (A25) into Eq. (A27) we obtain Eqs. (5). The summation over β in Eq. (A27) signifies that the Cooper pairs form spin singlets. The reason we treat separately the two parts of these singlets is that the long range magnetic impurities affect them differently in the Ising superconductor.

As discussed in the main text, the difference between the critical temperatures crucially depends on the range of the magnetic scattering. To illustrate this point we have plotted the critical temperature for the two spin orientations for the different range of the magnetic scattering, see Fig. 7. As is clear from these plots, the more delocalized the magnetic moments are the more pronounced is the effect.

Appendix B: The Γ model

The Γ pocket is singly connected and the analysis in this case is similar to the standard Abrikosov-Gor'kov theory. The momentum dependent spin splitting is written in the form of $\xi_{SO}\gamma(\hat{\mathbf{k}})$, and for the Γ -pocket we can take $\gamma(\hat{\mathbf{k}}) = \cos(3\phi_{\hat{\mathbf{k}}})$. The pair-breaking equation that controls the critical temperature, is almost identical to Eq. (A27),

$$\pi T \sum_{\omega_n} \left[\frac{\psi_0}{|\omega_n|} - \frac{i}{2} \sum_{\beta} \beta \langle f_2^{(\beta)}(\hat{\mathbf{k}}) \rangle_{\hat{\mathbf{k}}} \right] = \psi_0 \ln \left(\frac{T_{c0}}{T_c} \right), \quad (\text{B1})$$

where, as before $\langle \dots \rangle$ stands for the averaging over the directions, $\hat{\mathbf{k}}$, and the index $\beta = 1(-1)$ refers to Cooper pairs with the $\uparrow\downarrow$ ($\downarrow\uparrow$), respectively. In contrast to the

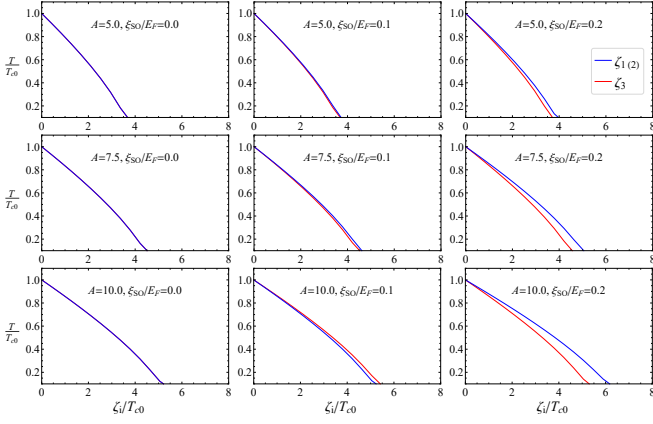


FIG. 8. The critical temperatures for the same set of parameters as in Fig. 7 for the Γ model. The calculation is done by numerically solving Eqs. (B1) and (B2) of the Fredholm type without resorting to the isotropic approximation.

$K(K')$ model the valley index is omitted.

The two functions $f_2^{(\pm 1)}(\hat{\mathbf{k}})$ satisfy the linear integral equations,

$$\begin{aligned} & \zeta_3 \left\langle \left(f_2^{(\beta)}(\hat{\mathbf{k}}') + f_2^{(\beta)}(\hat{\mathbf{k}}) \right) \mathcal{P}(\mathbf{q}_{\beta\beta}) \right\rangle_{\hat{\mathbf{k}}'} \\ & - (\zeta_1 + \zeta_2) \left\langle \left(f_2^{(\beta)}(\hat{\mathbf{k}}') - f_2^{(\beta)}(\hat{\mathbf{k}}) \right) \mathcal{P}(\mathbf{q}_{\beta\beta}) \right\rangle_{\hat{\mathbf{k}}'} \\ & = -|\omega_n| f_2^{(\beta)}(\hat{\mathbf{k}}) - \beta i \psi_0. \end{aligned} \quad (\text{B2})$$

which parallels Eq. (A23b). As before, $\Delta \mathbf{k}_{\beta\beta'}$ is the mo-

mentum change of an electron resulting from the elastic collision off a magnetic impurity.

In the spin-SU(2) invariant limit, the pair-breaking effect is isotropic with respect to the polarization of magnetic impurities. For finite SOC and for the long-range impurities it becomes anisotropic. For the spin-conserving processes, described by the terms $\propto \zeta_3$ in Eq. (B2), $\mathbf{q}_{\beta\beta}$, reaches zero for $\hat{\mathbf{k}} = \hat{\mathbf{k}}'$ as the both the initial and final states belong to the same Fermi surface. This is true for any initial momentum.

For the spin flip processes described by the terms $\propto \zeta_1, \zeta_2$, $\mathbf{q}_{\beta\beta}$ remains finite and on the order of ξ_{SO}/v_F . For this reason the T_c is anisotropic for both $K(K')$ and Γ models. Since in the Γ model the spin splitting vanishes along ΓM directions, the transferred momentum $\Delta \mathbf{k}_{\beta\beta}$ becomes small for the momenta along these symmetry lines. For this reason the T_c anisotropy is more pronounced for the $K(K')$ model than for the Γ model.

The SOC and more generally, the band structure introduces anisotropy in the problem, and the constant functions of $\hat{\mathbf{k}}$ are no longer solutions of the equation (B2). This linear integral equation of Fredholm type can be solved numerically, and the result of the numerical solutions for a particular Γ -model are shown in Fig. 8. These plots demonstrate that the general trend for increasing difference, $T_{c,\perp} - T_{c,\parallel}$ with the scattering range holds for the Γ and K -models alike. However, the comparison between the Figs. 7 and (8) shows that the effect for the K -model is stronger. The reason for this is the vanishing of the spin-orbit coupling along ΓM directions for the Γ -model.

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