



# Superconductivity in the transition metal dichalcogenide 4Hb-TaS<sub>2</sub>: magnetic memory and possible mechanisms

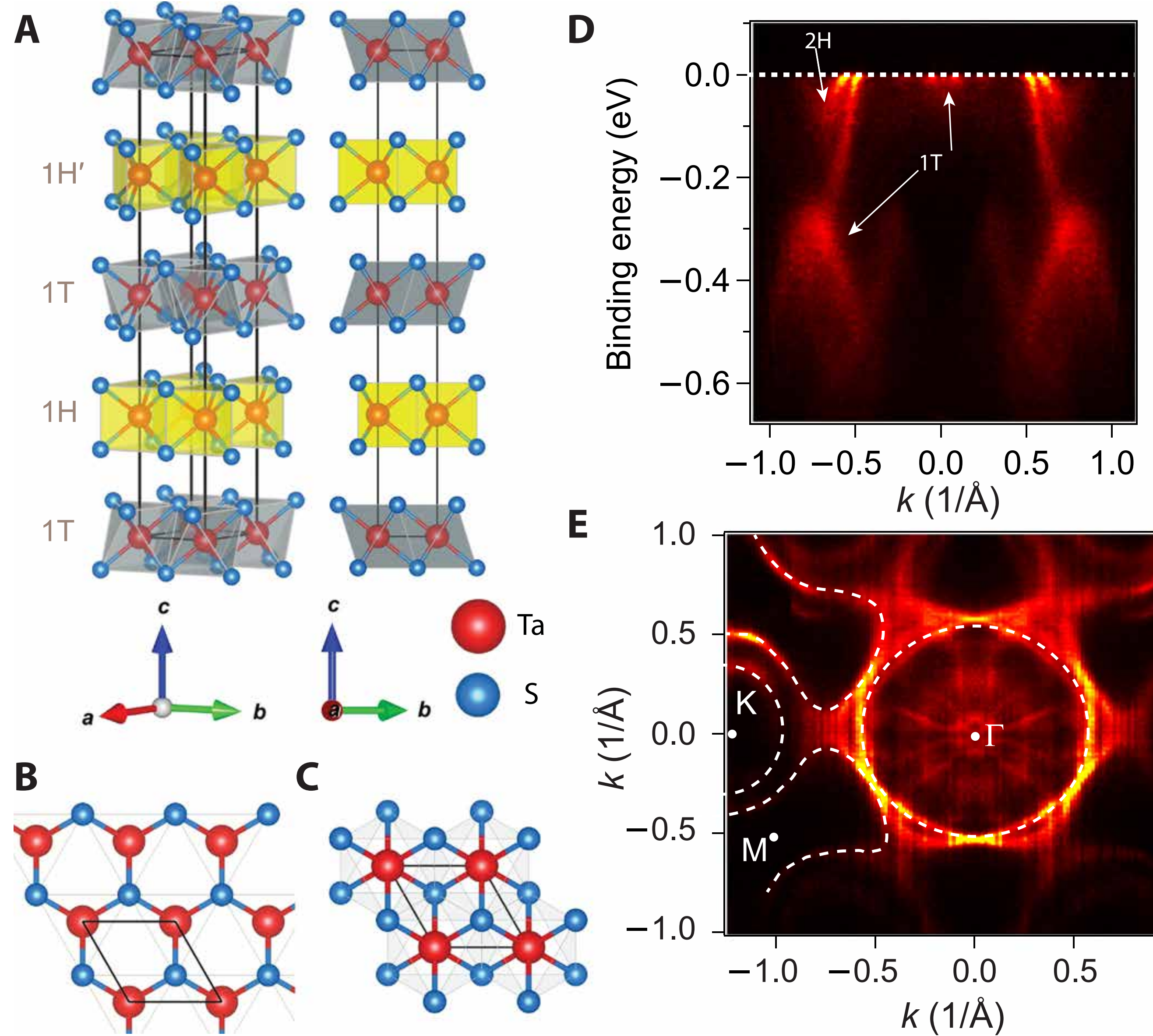
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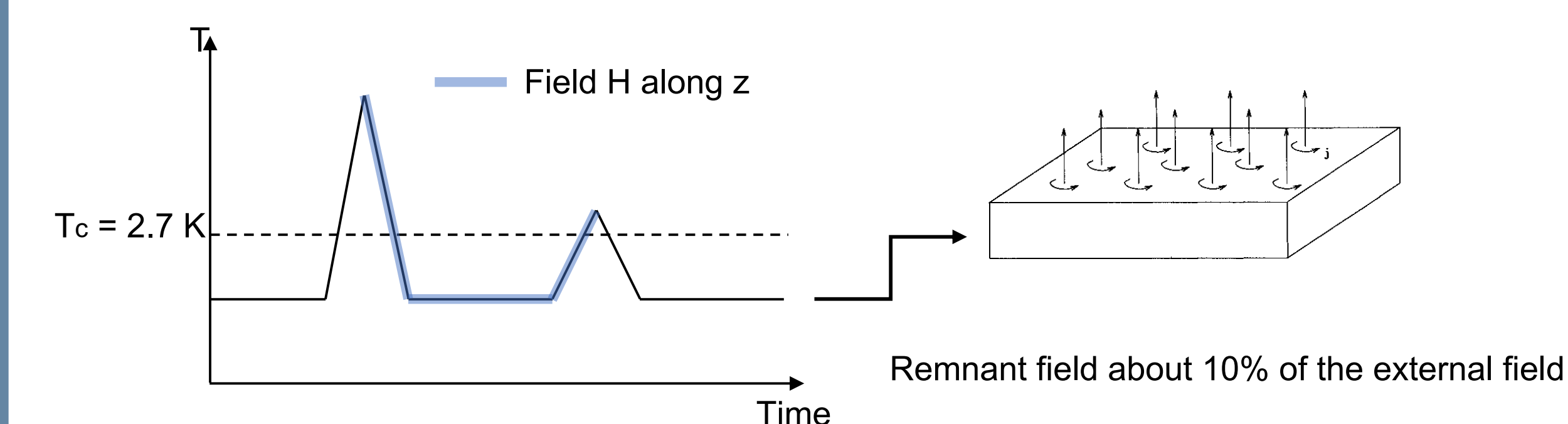
## ABSTRACT

A recent experiment on the transition metal dichalcogenide (TMD) 4Hb-TaS<sub>2</sub> reveals an unusual time-reversal-symmetry-breaking superconducting state that possesses a magnetic memory not manifest in the normal state. Here, we show that the normal state possesses very small magnetization due to almost cancellation of the spin and orbital parts. Based on the three-dimensional inversion symmetry and the material's band structure, we propose a simple mechanism that gives rise to the above unusual superconducting magnetic memory: magnetization amplification due to interlayer superconductivity in one of the spin species.

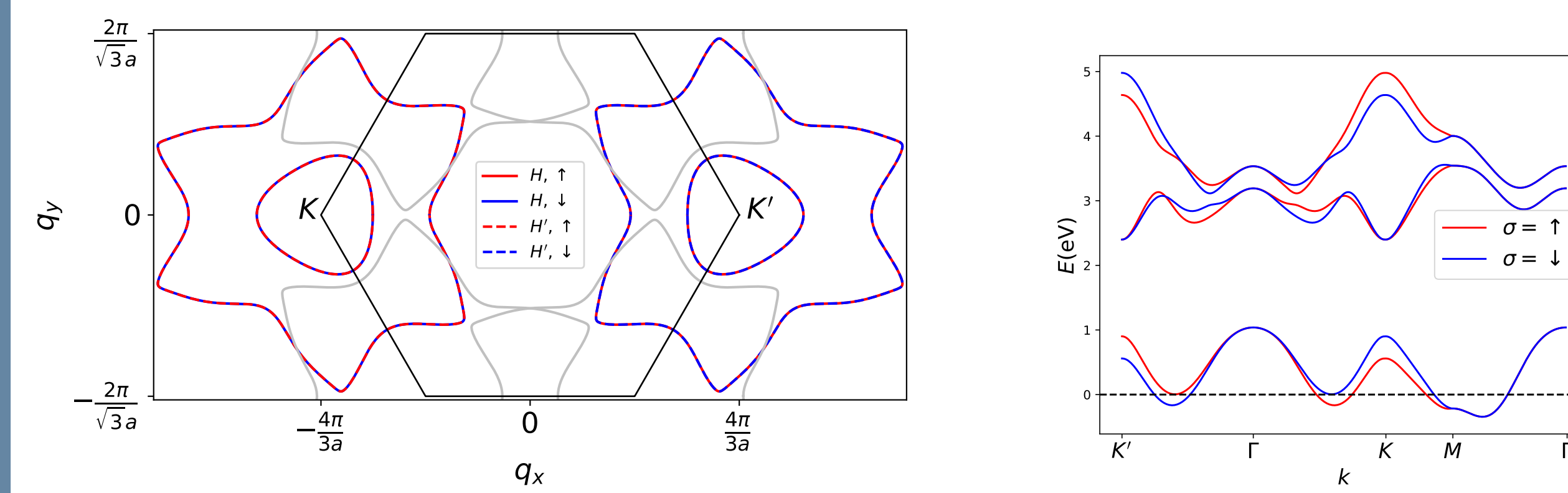
## EXPERIMENTAL OBSERVATION



- Superconductivity at  $T_c = 2.7$  K:  $T_c$  is accompanied with signatures of time-reversal symmetry breaking ( $\mu$ SR experiments) [1];
- FC-ZFC cycle: spontaneous vortices in the superconducting state [2];
- Magnetization in the metallic normal state:  $M$ - $H$  curve shows no hysteresis.



## MODELING THE NORMAL STATE

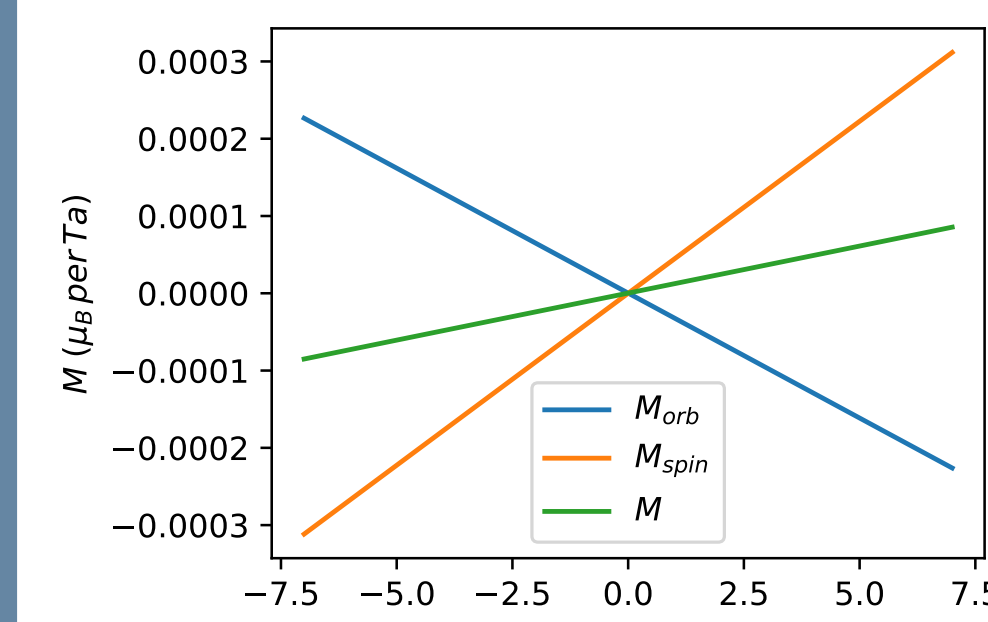


Starting point: a tight binding TMD Hamiltonian [3] with realistic parameters. The model has 6 bands ( $d_{x^2-y^2}, d_{xy}, d_{z^2}$  orbitals  $\times$  spin  $\sigma = \uparrow, \downarrow$ ), up to third-nearest neighbor hopping, with onsite spin-orbit coupling  $\mathcal{H}_{\text{soc}} = \lambda \hat{L}_z \hat{S}_z$ . Spins  $\uparrow$  and  $\downarrow$  are *decoupled*. The two bands across  $E_F$  have zero Chern number.

We calculate the total magnetization  $\mathbf{M} = M_z \hat{z}$  as a function of Zeeman field  $B \parallel \hat{z}$ . In absence of the field,  $\mathbf{M}$  for spin up and down cancel each other due to time reversal symmetry. The spin up  $M_z^\uparrow$  is the sum of the following three terms:

$$(M_{\text{spin},\uparrow}^z, M_{\text{orb,itin},\uparrow}^z, M_{\text{orb,loc},\uparrow}^z) = (0.2362g_s, -0.04168, 0.12318g_A) \mu_B/\text{Ta},$$

where  $g_{s,A}$  are the  $g$  factors for spin and orbital angular momentum, respectively. Interestingly, the orbital magnetization almost cancels the spin magnetization.



Summary: the applied field splits the spin degeneracy in the normal state. The magnetization can still be arbitrarily small due to the cancellation of orbital and spin moments, which potentially accounts for the absence of hysteresis in the  $M$ - $H$  curve for the normal state.

## SUPERCONDUCTING STATE: SYMMETRY ARGUMENTS

The Fermi surface location suggests two possible pairings

$$\underbrace{(\uparrow, \mathbf{H}, \mathbf{k}) \leftrightarrow (\downarrow, \mathbf{H}, -\mathbf{k})}_{\text{opposite spin, intralayer pairing}} \quad \text{or} \quad \underbrace{(\uparrow, \mathbf{H}, \mathbf{k}) \leftrightarrow (\uparrow, \mathbf{H}', -\mathbf{k})}_{\text{same spin, interlayer pairing}}$$

Due to the splitting of spin up and down bands, the spin up and down Fermi surfaces are no longer of the same shape, suppressing intralayer pairing.

We notice that a symmetry classification of the gap function is possible [4]. Symmetry group is  $D_{6h}$  which contains  $p$ , the 3D inversion centered on the 1T layer. One may look for unconventional superconductivity in the " $E_g$ " and " $E_u$ " irreps of the classification tables, which may inform the observation of Ref. [1].

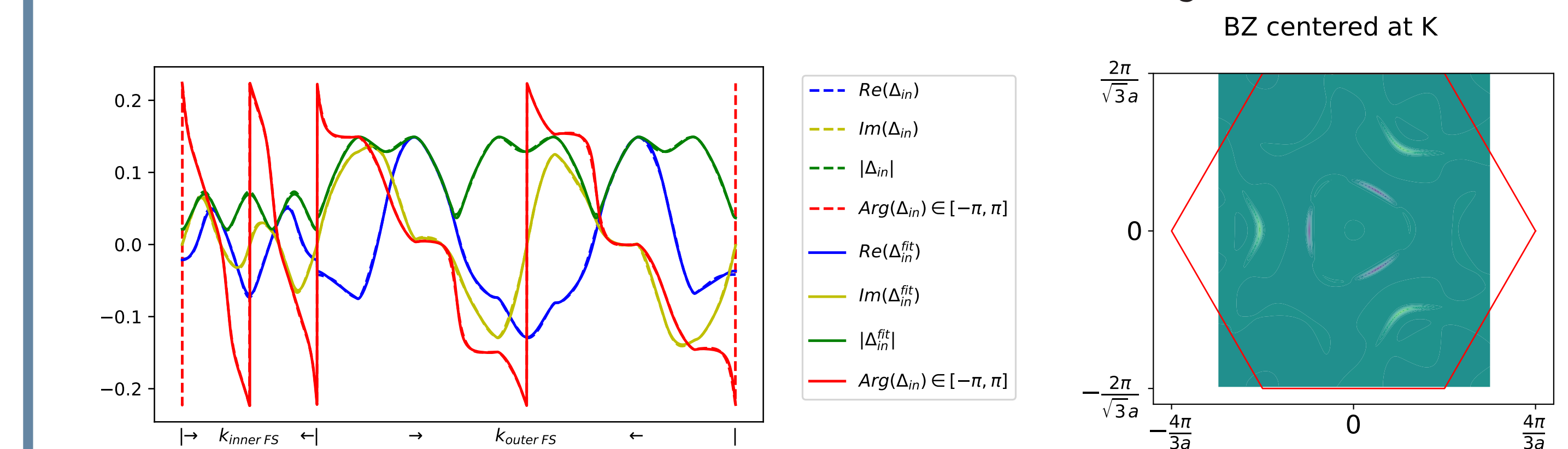
In the following, we assume *interlayer pairing*  $c_{\uparrow, \mathbf{H}, \mathbf{k}}^\dagger c_{\uparrow, \mathbf{H}', -\mathbf{k}}^\dagger$ . One immediate consequence of this pairing is that it must *break* the 3D inversion  $p$ , since any such term is odd under  $p$ . However, a modified 3D inversion of  $p'$  can be preserved, and can help *stabilize* the vortices as a normal  $p$  does.

## BCS SOLUTION AND MAGNETIZATION

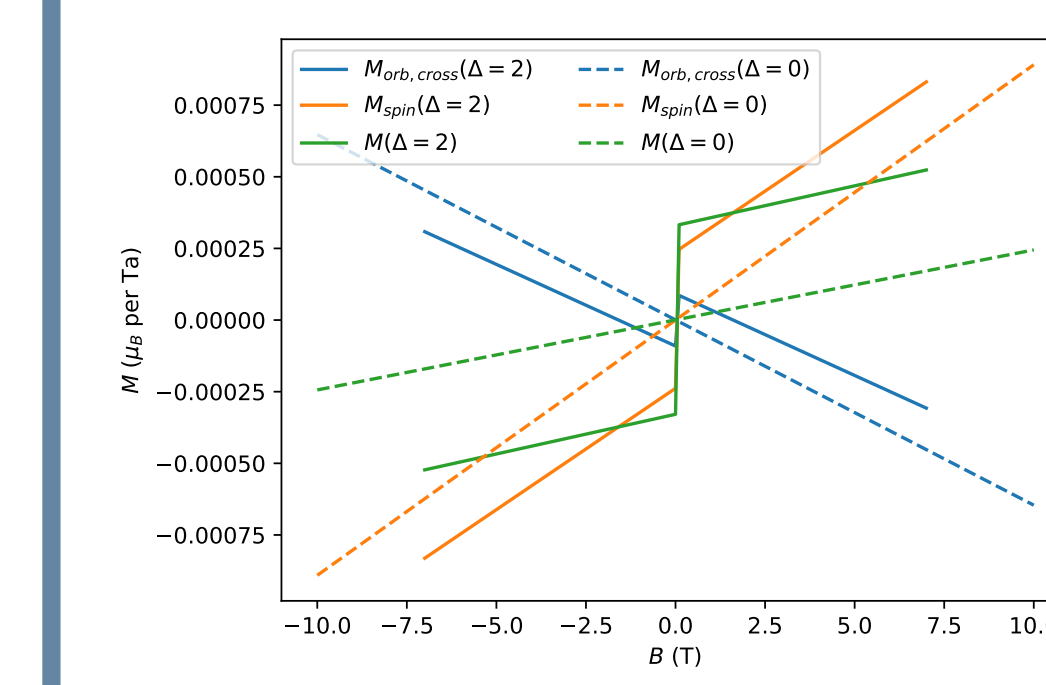
We solve the linearized gap equation

$$\Delta_{\mathbf{k}} = - \int \frac{d^2 k'}{(2\pi)^2} V(\mathbf{k} - \mathbf{k}') \underbrace{(\langle u_{\mathbf{k}, \uparrow, \mathbf{H}} | u_{\mathbf{k}', \uparrow, \mathbf{H}} \rangle)^2}_{\mathcal{M}_{\mathbf{k}, \mathbf{k}'}} \frac{\tanh(\frac{\epsilon_{\mathbf{k}', 1}}{2T})}{2\epsilon_{\mathbf{k}', 1}} \Delta_{\mathbf{k}'}$$

For simplicity, we assume a constant attractive interaction  $V(\mathbf{k}) = V < 0$ . The eigenvector corresponding to the maximum eigenvalue of the matrix  $\mathcal{M}_{\mathbf{k}, \mathbf{k}'}$  gives solution to the gap function. We further approximate the gap function by short-range lattice interlayer pairings, as shown below. We emphasize that while the (gauge noninvariant) gap function appears with a winding of  $4\pi$  on the FSs the gauge invariant quantity has zero winding. In this sense, the gap solution is "s-wave" in nature, and the BdG Hamiltonian has zero winding.



We note that the superconducting temperature  $T_c$  is a monotonous function of chemical potential  $\mu = \frac{1}{2} \mu_{\text{BG}} \sigma B$ . This means that a  $+\hat{z}$  ( $-\hat{z}$ ) direction field favors  $\sigma = \uparrow$  ( $\sigma = \downarrow$ ) BCS state. We postulate that *one spin flavor forms into interlayer cooper pairs, while the other stays in the normal state*.



Next, we compute the magnetization in the BCS state [5], assuming only one spin flavor forms Cooper pairs. The magnetization is "amplified" in the BCS state for a single spin; the hysteresis and the magnitude of the magnetization are consistent with the remnant field in the experiment.

## REFERENCES

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- [4] Fischer, Mark H., and Jun Goryo: *Symmetry and gap classification of non-symmorphic SrPtAs*, Journal of the Physical Society of Japan 84.5 (2015): 054705.
- [5] Robbins, Joshua, James F. Annett, and Martin Gradhand: *Theory of the orbital moment in a superconductor*, Physical Review B 101.13 (2020): 134505.

## ACKNOWLEDGEMENTS

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