

Zero-bias conductance peak in detached flakes of superconducting 2H-TaS₂ probed by STS

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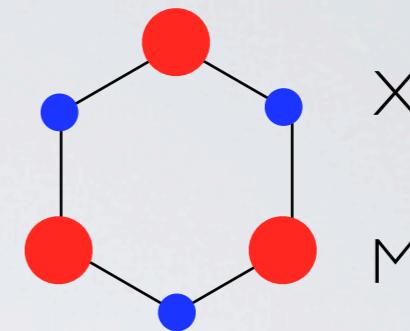
Instituto de Ciencia Molecular (ICMol), Universidad de Valencia, Paterna, Spain

J.A. Galvis et al., Phys. Rev. B **89**, 224512 (2014)

Transition metal dichalcogenides

layered materials: van der Waals forces between layers

each layer: three atomic planes



$X = S, Se$

$M = Ta, Nb$ metallic

$M = W, Mo$ semiconducting

2H polytype

Report **STM** measurements on single layer of **2H-TaS₂**

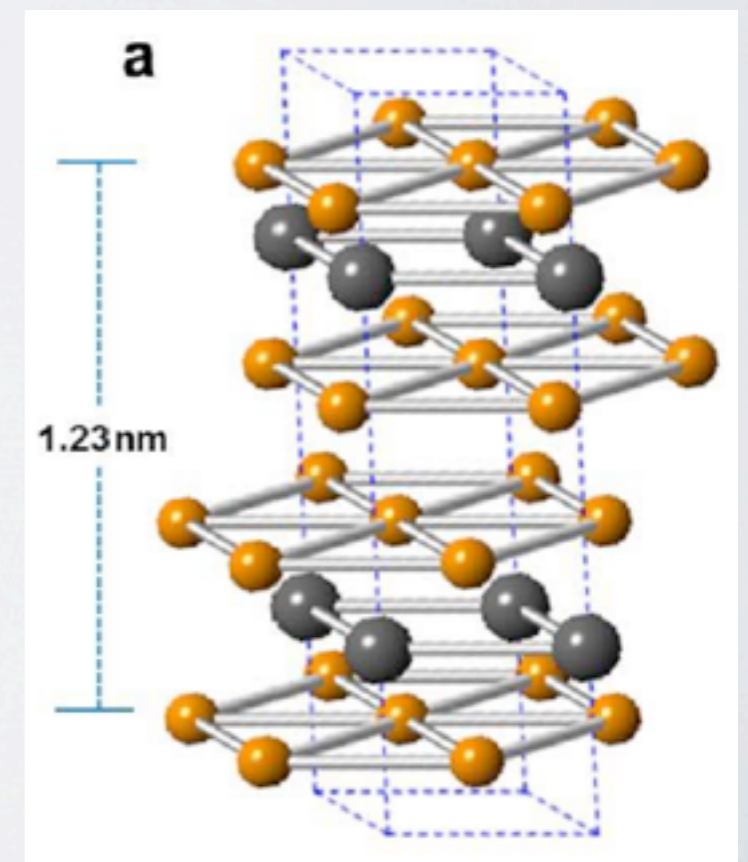
Fermi surface has a strong Ta character

5 d orbitals from Ta

2x3 p orbitals from S

strong spin-orbit

2H polytype
parity symmetric

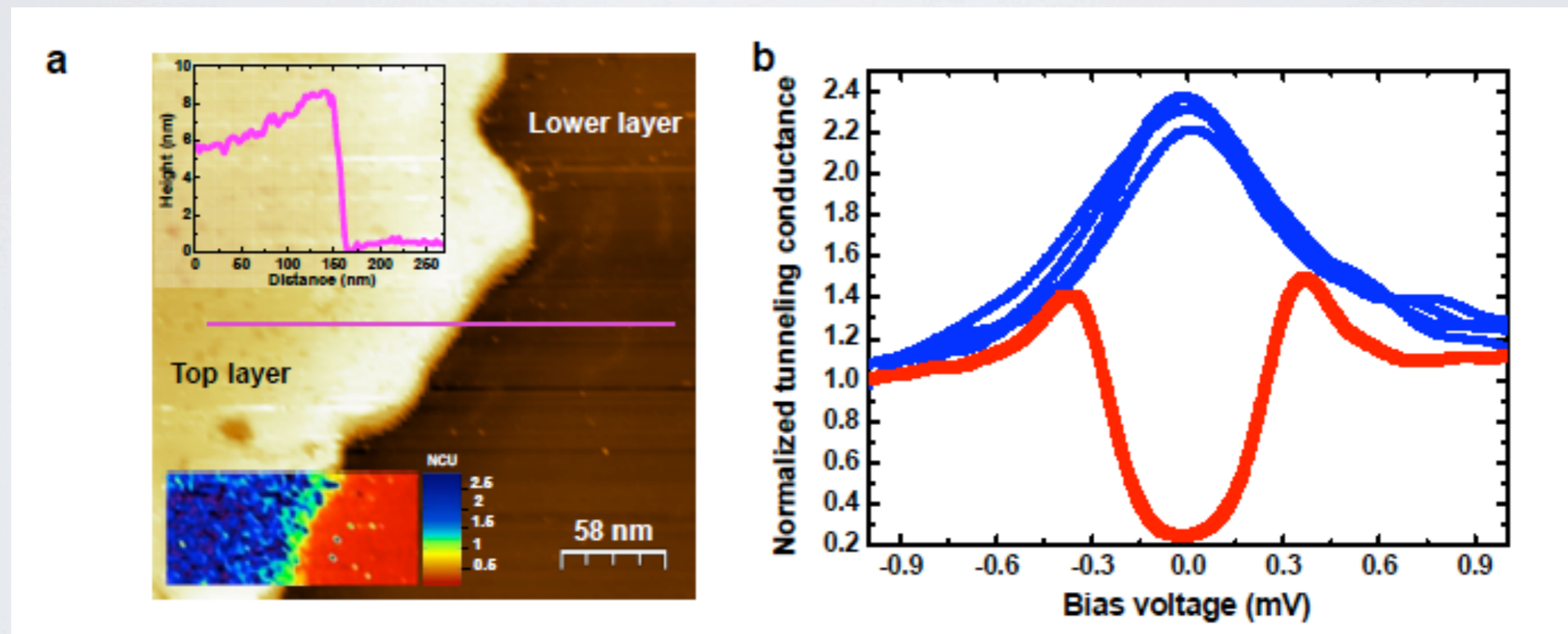


STM measurement of surface of 2H-TaS₂

scanning the **bulk** surface: **BCS like gap**

scanning the **single layer** surface: **Zero Bias Conductance Peak**

not compatible with BCS theory



Similar results for 2H-TaSe₂

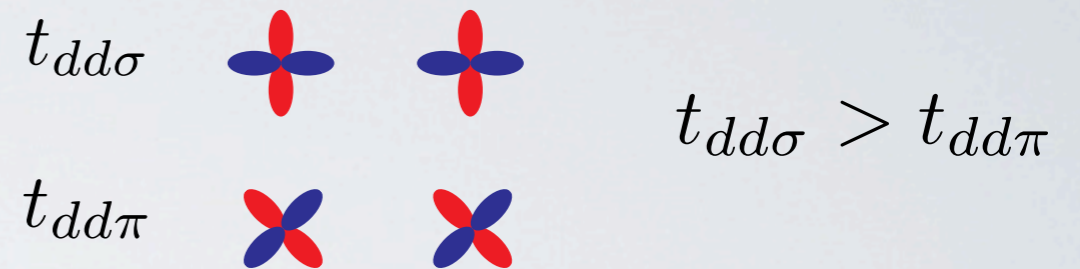
J. A. Galvis et al., Phys. Rev. B **87**, 094502 (2013)

Tight binding model

two Ta orbitals on a triangular lattice $d_{x^2-y^2}$ d_{xy}

effective model:

nearest-neighbour hopping



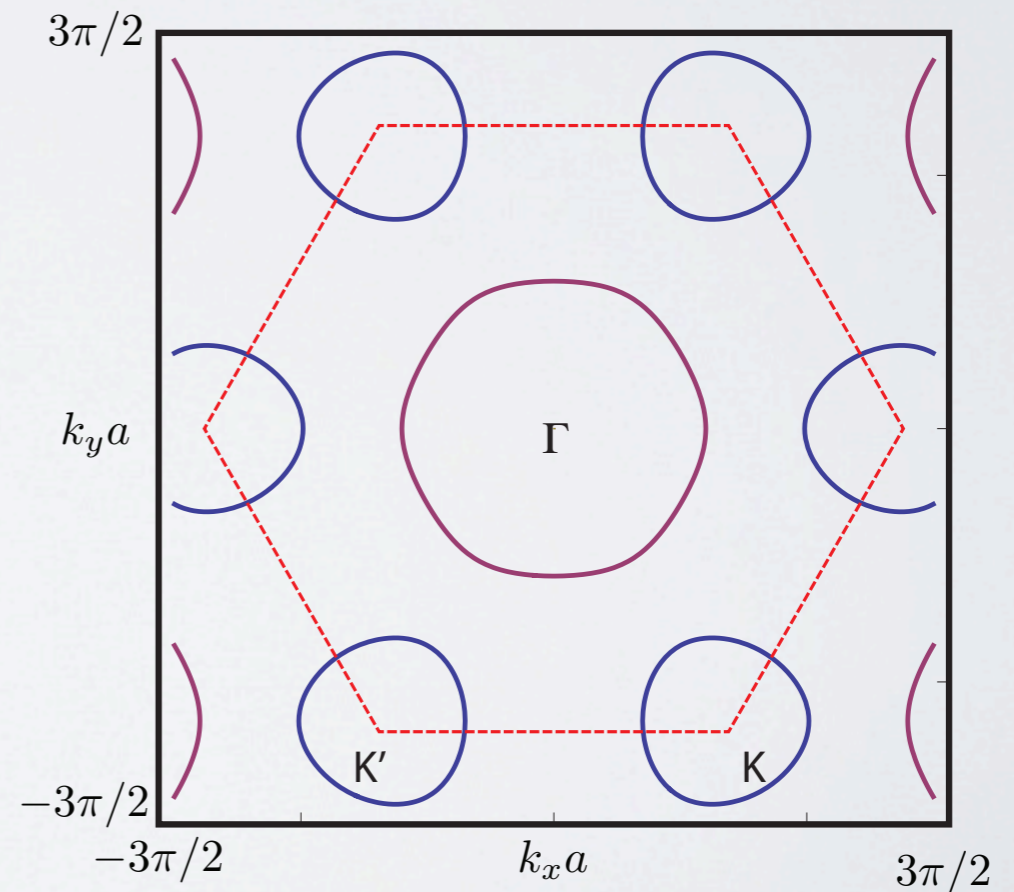
$$H_0 = - \sum_{\mathbf{R},\sigma} \sum_{i=1}^3 c_{\mathbf{R},\sigma}^\dagger h_i c_{\mathbf{R}+\mathbf{a}_i,\sigma} + \text{H.c.}$$

$$\mathcal{H}_{\mathbf{k}}^0 = -2 \sum_{i=1}^3 h_i \cos(\mathbf{k} \cdot \mathbf{a}_i)$$

two orbitals \longrightarrow two bands Γ \mathbf{K}

\mathbf{K} \mathbf{K}' inequivalent points in the BZ

\longrightarrow **three bands**



Possible odd-momentum superconductivity

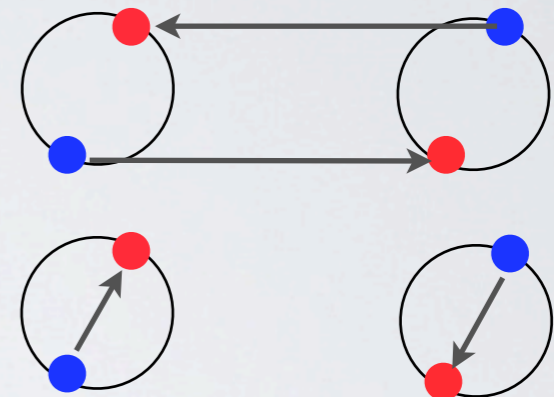
Fermi surface has a strong Ta 5d character

non-negligible role of Coulomb interaction

Strong K, K' interband scattering due to short range Coulomb repulsion

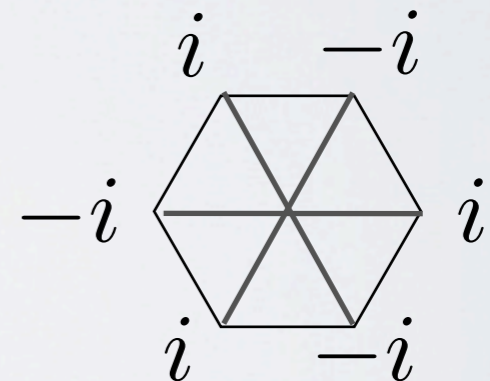
favors a odd-momentum gap

$$\Delta_{K'} = -\Delta_K$$



tight-binding imaginary nearest neighbour pairing

$$H_{SC} = -i\delta \sum_{\mathbf{R}, \alpha} \sum_{s=\pm, j=1}^3 s(-1)^j c_{\mathbf{R}\alpha\uparrow}^\dagger c_{\mathbf{R}+s\mathbf{a}_j, \alpha\downarrow}^\dagger + \text{H.c.}$$



$$\Delta_{\mathbf{k}} = 2\delta \sum_{i=1}^3 (-1)^i \sin(\mathbf{k} \cdot \mathbf{a}_i)$$

odd-momentum gap

$$\Delta_{-\mathbf{k}} = -\Delta_{\mathbf{k}}$$

Nodal odd-momentum superconductivity

Bogoliubov de Gennes Hamiltonian $H_{\text{BdG}} = \frac{1}{2} \sum_{\mathbf{k}} \psi_{\mathbf{k}}^\dagger \mathcal{H}_{\mathbf{k}}^{\text{BdG}} \psi_{\mathbf{k}}$

Nambu spinor $\psi_{\mathbf{k}} = \begin{pmatrix} c_{\mathbf{k}} \\ \mathcal{T} c_{\mathbf{k}} \end{pmatrix}$

time-reversal operator $\mathcal{T} = i s_y \hat{K}$

$$\mathcal{H}_{\mathbf{k}}^{\text{BdG}} = (\mathcal{H}_{\mathbf{k}}^0 - \mu) \tau_z + \Delta_{\mathbf{k}} s_z \tau_x$$

K pocket Δ

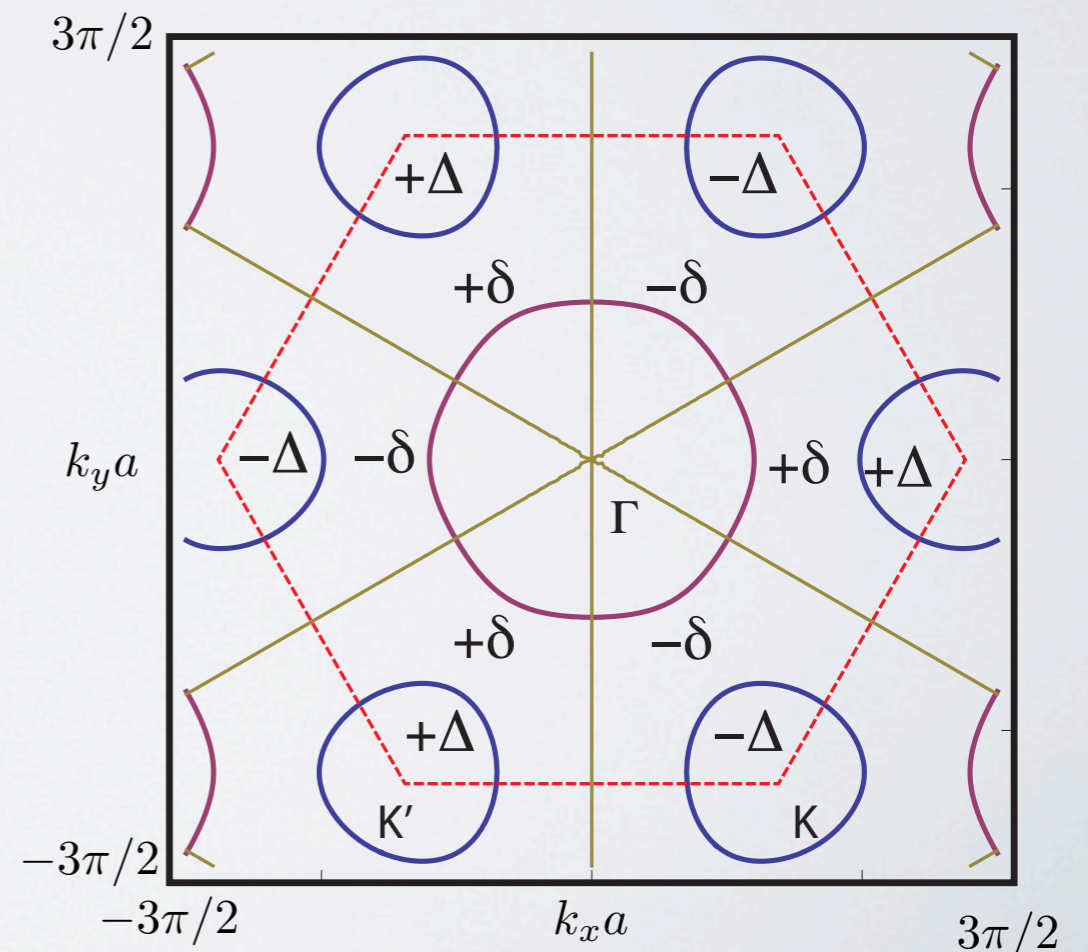
K' pocket $-\Delta$

Γ pocket **nodal** δ

nodal gap induced by the K, K'

six nodes: symmetry robustness

triplet f-wave pairing



STM local density of states

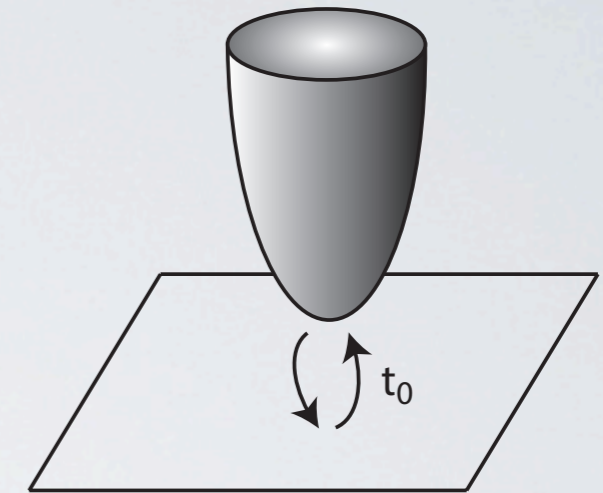
usually the STM measures the unperturbed density of states

Bardeen theory

$$\frac{dI}{dV} \propto \int d\omega \sum_{\lambda, \sigma} |T_\lambda|^2 A_\sigma(\lambda, \omega) f'(\omega - eV)$$

perturbative in tunneling

unperturbed
spectral function



local DOS

$$|T_\lambda|^2 = \sum_{\rho} |M_{\lambda\rho}|^2 A_{\text{tip}}(\rho, \omega)$$

$$A_\sigma(\lambda, \omega) = -\frac{1}{\pi} \text{Im} G_\sigma(\lambda, \omega + i0^+)$$

$$\frac{dI(\mathbf{r})}{dV} \propto \rho(eV, \mathbf{r}) = -\frac{1}{\pi} \sum_{\sigma} \text{Im} G_\sigma(\mathbf{r}, \mathbf{r}; eV + i0^+)$$

Effective Dirac BdG Hamiltonian

Expand BdG Hamiltonian around nodal points

$$t_{dd\sigma} \gg t_{dd\pi}$$

$$\mathcal{H}_Q^{\text{BdG}} \simeq v_F k_y \tau_z + v_\Delta k_x \tau_x$$

$$\epsilon_Q(\mathbf{k}) \simeq \sqrt{v_\Delta^2 k_x^2 + v_F^2 k_y^2}$$

$$v_F \simeq a t_{dd\sigma}$$

$$v_\Delta \simeq a \delta$$

retarded Green'sfunction

$$g^r(\epsilon) \simeq \frac{N_f A_c}{2\pi v_F v_\Delta} \left[-2\epsilon \ln \frac{\delta}{|\epsilon|} - i\pi |\epsilon| \right]$$

$$N_f = 12$$

δ cutoff of the linear dispersion

6 spin-degenerates nodes

$$\rho(\epsilon) \sim \frac{N_f A_c}{2\pi v_F v_\Delta} |\epsilon|$$

V-shaped gap around the Fermi energy

analogous to **graphene**

this is not what is measured

Possible explanation

within the theoretical model **two** assumptions: $\left\{ \begin{array}{l} \text{nodal odd-momentum superconductivity} \\ \text{perturbative tip-sample coupling} \end{array} \right.$

no magnetic impurities \rightarrow simple s-wave BCS superconductivity **cannot** explain a ZBCP

strong short range interaction \rightarrow odd-momentum superconductivity

Can we relax the perturbative tip-sample coupling assumption?

two gaps: $\left\{ \begin{array}{ll} \text{K} & \text{K}' \text{ pocket } \Delta & -\Delta \\ \Gamma & \text{pocket } \delta & \text{nodal} \end{array} \right. \quad \delta \ll \Delta$

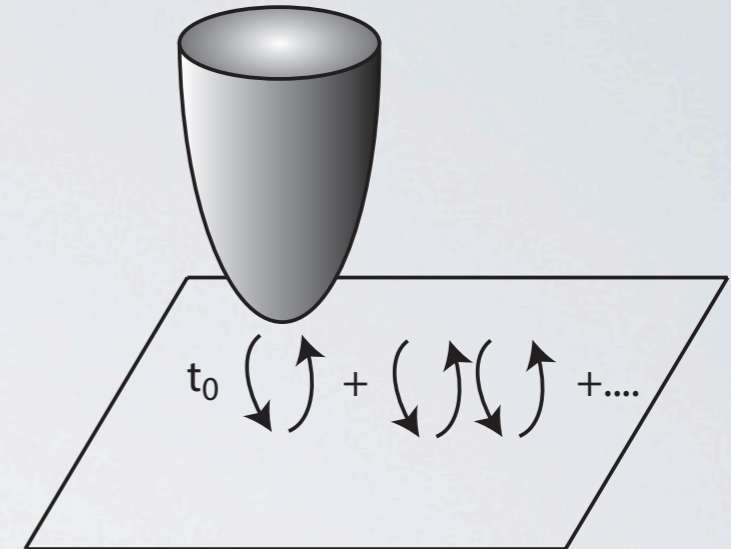
tip-sample coupling $\left\{ \begin{array}{ll} \text{K} & \text{K}' \text{ perturbative} \\ \Gamma & \text{non-perturbative} \end{array} \right. \rightarrow \text{tip-modified local DOS}$

Non-perturbative tip-sample coupling

assume point-like tunneling t_0

SC Green's function $\hat{g}_{\text{sc}}(z) = \sum_{\mathbf{k}} (z - \mathcal{H}_{\mathbf{k}}^{\text{BdG}})^{-1}$

odd gap $\Delta_{-\mathbf{k}} = -\Delta_{\mathbf{k}}$ $\sum_{\mathbf{k}} \frac{\Delta_{\mathbf{k}}}{E_{\mathbf{k}}} = 0$



No Andreev current

analogous to tunneling to a **semiconductor**

analogous to tunneling to a **graphene**

differential conductance $\sigma(\omega) = \frac{e^2}{h} \frac{4\pi^2 t_0^2 \rho_{\text{tip}}(\omega - eV) \rho_{\text{sc}}(\omega)}{|1 - t_0^2 g_{\text{tip}}(\omega - eV) g_{\text{sc}}(\omega)|^2}$

tip self-energy $\Sigma_{\text{tip}}(\omega) = t_0^2 g_{\text{tip}}(\omega) \simeq -i\pi t_0^2 \rho_{\text{tip}}$

Resonant behaviour

$$1 - \Sigma_{\text{tip}} g_{\text{sc}}(\Omega) = 0$$

retarded Green's function defined in the upper half of complex energy plane

$$g_{\text{sc}}(z) = Cz \ln(-iz)$$

$$z = \epsilon/\delta$$

$$1 + i\lambda z \ln(-iz) = 0$$

$$\lambda = t_0^2 \rho_{\text{tip}} C \quad \text{effective coupling}$$

$$C = \frac{N_f A_c \delta}{\pi v_\Delta v_F}$$

$$z = ix \quad \text{purely imaginary resonance}$$

$$x \ln x = 1/\lambda \quad \text{for strong coupling solution compatible with cutoff}$$

broad resonance at zero energy

compatible with experimental observation

Zero Bias Conductance Peak

the tip-sample coupling is usually perturbative

effective coupling $\lambda = N_f \tilde{\lambda}$

$$\rho_{\text{sys}} = A_c / av_F$$

microscopic coupling $\tilde{\lambda} = t_0^2 \rho_{\text{tip}} \rho_{\text{sys}}$

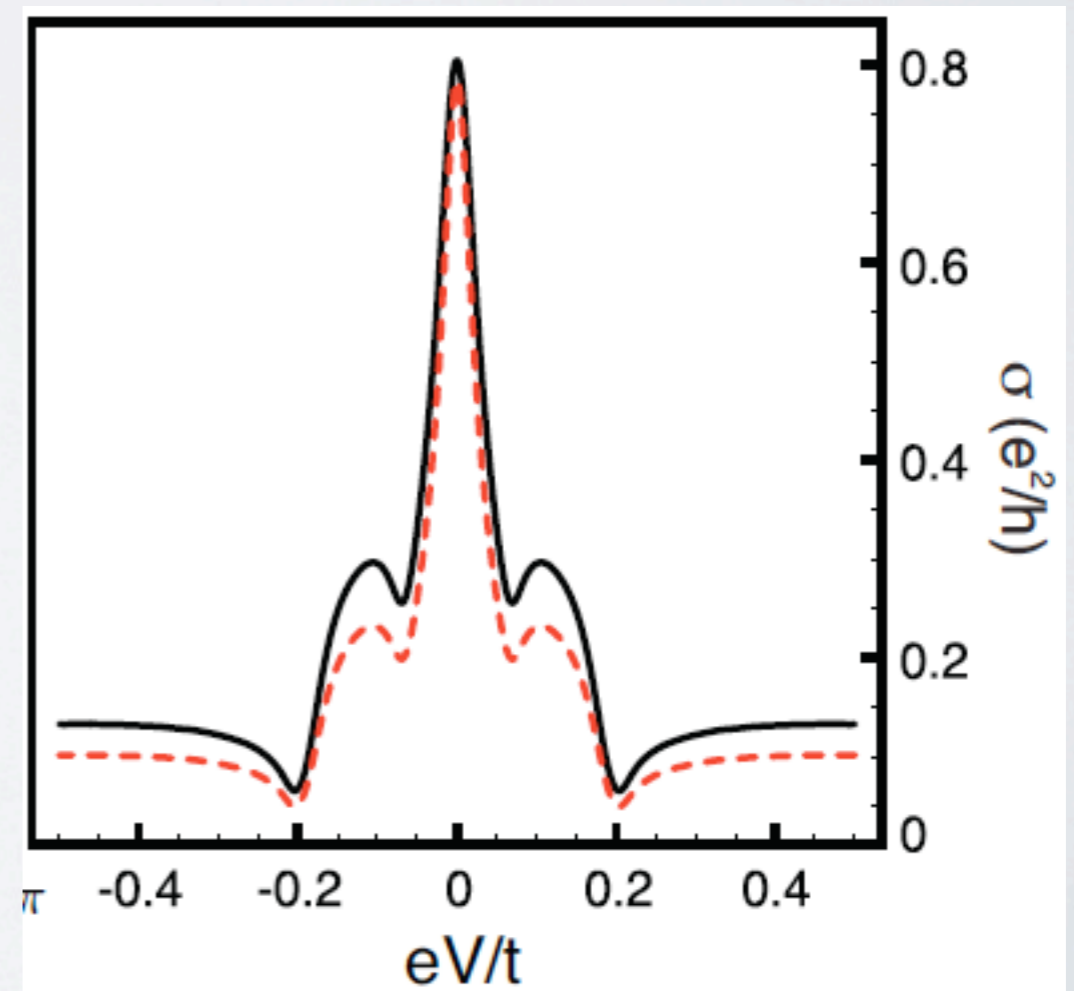
$$\tilde{\lambda} \ll 1 \quad \text{perturbative}$$

for a large N the **effective coupling** can become **non-perturbative**

conductance with the full tight-binding

valid at all energies

broad ZBCP



Summary and Conclusions

experimentally observed Zero Bias Conductance Peak in single layer 2H-TaS₂

ZBCP found in a large area

ruled out any local mechanism such as magnetic impurity

non-compatible with BCS-like theory

strong short range Coulomb repulsion can induce odd-parity gap at K and K'

nodal induced gap on the Gamma pocket

perturbative STM cannot explain measurements

on the Gamma pocket a **weak tip-sample coupling can become non-perturbative**