



# Andreev reflection and subgap conductance in monolayer $\text{MoS}_2$ ferromagnet/s and $d$ -wave superconductor junction

H. Goudarzi\*, M. Khezerlou, S.F. Ebadzadeh

Department of Physics, Faculty of Science, Urmia University, Urmia, P.O. Box: 165, Iran

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## ABSTRACT

The accurate and proper form of electron-hole excitations and corresponding Dirac-like spinors of superconducting monolayer molybdenum disulfide are exactly obtained. Andreev reflection and resulting subgap conductance in a  $\text{MoS}_2$ -based ferromagnet-superconductor (F/S) junction are particularly calculated in terms of dynamical characteristics of structure. Due to the spin-splitting energy gap in the valence band and also nondegenerate  $K$  and  $K'$  valleys, the ferromagnetic exchange energy  $sh$  can cause a distinct behavior of Andreev reflection process between spin-up and spin-down charge carriers in the different valleys. In order to occur the retro Andreev reflection, the chemical potential is necessarily fixed in a determined range. Given here one-particle superconducting bispinors enable us to explicitly involve the anisotropic superconducting gap  $\Delta_S$  under electron-hole conversion, i.e., taking place in  $d$ -wave asymmetry. Dependence of the Andreev process on the electron incidence angle at the interface is explicitly explored in the presence of such superconducting pair potential.

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## 1. Introduction

Two-dimensional condensed matters such as graphene [1] and monolayer molybdenum disulfide (ML-MDS) [2–4] including Dirac-like charge carriers can present itself as a capable structure to observe distinct transport properties resulting from Andreev reflection (AR) or Klein transmission. By the Blonder-Tinkham-Klapwijk [5] formalism, the peculiar Andreev process results in a finite conductance in a normal/superconductor junction at the electron excitations below the superconducting gap  $\Delta_S$ . Another interesting feature of AR has been proposed by Beenakker [6] as specular AR, when a N/S proximity junction is realized in graphene, where an electron from the conduction band is reflected as a hole in the valence band, so that the reflection angle is inverted with respect to the incidence. This effect can be justified by the dependence of the subgap Andreev conductance on bias voltage (electron excitation). Recently, the AR was studied at the interface of ML-MDS superconductor/normal metal [7], where the authors show the p/n-doping effect (the magnitude of the chemical potential in the normal region relative to the superconductor region) on the retro AR. This can be of much attention, since charge carriers exhibit either the electron-like or hole-like quasiparticles belonging to two inequivalent nondegenerate  $K$  and  $K'$  valleys. Comparing with graphene, such attention for ML-MDS is highlighted by some distinct features of  $\text{MoS}_2$ : i) appearance of direct band-gap in low-energy band excitations in the visible frequency range ( $\approx 0.95$  eV), ii) strong spin-orbit coupling (SOC) resulted from heavy metal atom of  $Mo$ , iii) breaking the valley degeneracy by the valley-contrasting spin splitting

\* Corresponding author.

E-mail addresses: [h.goudarzi@urmia.ac.ir](mailto:h.goudarzi@urmia.ac.ir), [goudarzia@phys.msu.ru](mailto:goudarzia@phys.msu.ru) (H. Goudarzi), [m.khezerlou@urmia.ac.ir](mailto:m.khezerlou@urmia.ac.ir) (M. Khezerlou).

( $\approx 0.1 - 0.5$  eV) caused by inversion symmetry breaking [4,8,9]. In this paper, firstly we, in particular, investigate the explicit dependence of Andreev process on the electron incidence angle in the proximity-induced  $\text{MoS}_2$  ferromagnetic and superconductor F/S and N/S junctions (see Fig. 1) by determining the allowed chemical potential of F or N regions due to the significant spin-splitting energy in the valence band. To this end, we obtain the explicit expression for the ML-MDS superconducting electron-hole excitations and corresponding Fermi wavevector, which enables us to find appropriate form of corresponding Dirac-Bogoliubov-de Gennes (DBdG) spinors. We show that these spinors are fundamentally different from those obtained in the previous works [7,10], so that we are allowed to evaluate the difference of superconducting gap under electron-hole converting, taking place in  $d$ -wave superconductivity [11–13]. Secondly, we focus on the F/S structure, because of the exchange splitting energy  $h$  of F metal may induce a large spin-splitting of  $K'$  valley in the valence band. Actually, it results in a novel behavior of pseudo-relativistic Klein tunneling giving rise to a conductance difference between spin-up and spin-down charge carriers and resulting magnetoresistance [14]. The same structure with graphene was studied in Ref. [15].

Moreover, the proximity-induced superconductivity and ferromagnetism in  $\text{MoS}_2$  can be experimentally achieved [16–25]. Recently, the physics of spin and valley coupling [9], and ferromagnetic/superconductor/ferromagnetic [26] junction have been studied in the ML-MDS structures. Further, the contribution of Schrodinger-like terms [27] (topological and mass asymmetry between electron and hole) are taken into account in the Dirac-like one-particle superconductor excitations. In addition, we investigate the effect of anisotropic  $d$ -wave pairing  $d_{x^2-y^2}$  on the resulting AR in the Hamiltonian of ML-MDS, because the sign of such pair potential  $\Delta_S^{e(h)} = \Delta_0 \cos(2\theta_S^{e(h)} - (+)2\alpha_S)e^{i\phi}$  may be changed by electron-hole conversion. This can lead to form the zero energy states in the relative Josephson junction [28] and corresponding zero-bias Andreev conductance. The superconducting wavefunctions obtained by us allow to explicitly exert this feature in the quasiparticle states.

This paper is organized as follows. Sec. 2 is devoted to present the proposed model and formalism to obtain the exact form of  $\text{MoS}_2$  superconducting dispersion energy and corresponding spinors. The normal and Andreev reflection coefficients are found by matching the wavefunctions at the interface. The numerical results of AR and resulting tunneling conductance are presented considering the strong spin-valley effect caused by ferromagnetic exchange field and also asymmetric superconducting order, and their main characteristics are discussed in the sections 3 and 4. Finally, we close with a brief summary.

## 2. Theoretical formalism

A typical F/S structure on top of a ML-MDS sheet is introduced with the configuration that the ferromagnetic and superconductor regions are extended from  $x = -\infty$  to  $x = 0$  and from  $x = 0$  to  $x = +\infty$  for all  $y$ , respectively as shown in Fig. 1. The low-energy band structure of ML-MDS can be described by the modified Dirac Hamiltonian. This Hamiltonian in addition to the first order term of momentum for 2D massive fermions, contains the quadratic terms originated from the difference mass between electron and hole  $\alpha$  and also topological characteristic  $\beta$ . The strong spin-orbit coupling causes the spin splitting at the valence band for different valleys. In the presence of an exchange field  $h$  and superconducting gap induced by proximity effect, the Dirac-Bogoliubov-de Gennes (DBdG) Hamiltonian is given by:

$$\mathcal{H} = \begin{pmatrix} h_0 - E_F + U(x) - sh & \Delta_S \\ \Delta_S^* & -h_0 + E_F - U(x) - sh \end{pmatrix}, \quad (1)$$

where  $h_0 = \hbar v_F k \cdot \sigma_\tau + \Delta\sigma_z + \lambda s\tau(1 - \sigma_z) + \hbar^2 |k|^2 / 2m_0(\alpha/2 + \beta/2\sigma_z)$ , and  $\sigma_\tau = (\tau\sigma_x, \sigma_y)$  are the Pauli matrices. The spin-up and spin-down is labeled by  $s = \pm 1$ , and valley index  $\tau = \pm 1$  denotes the  $K$  and  $K'$  valleys. The bare electron mass is  $m_0 = 0.05 \times 10^{-10}$  (eVs<sup>2</sup>/m<sup>2</sup>), topological and mass difference band parameters are evaluated by  $\beta = 2.21$  and  $\alpha = 0.43$ , respectively.  $\Delta$  is the direct band gap,  $\lambda \approx 0.04$  eV and  $v_F = 0.53 \times 10^6$  m/s denote the spin-orbit coupling and Fermi velocity, respectively. The electrostatic potential  $U(x)$  gives the relative shift of Fermi energy in the F and S regions. The superconducting gap is presented by  $\Delta_S$ , which in the  $d$ -wave symmetry case, as mentioned in the previous section it is parameterized by the electron incidence angle (with respect to the perpendicular direction to the interface)  $\theta_s$  in the S region and orbital rotated angle  $\alpha_s$ , respectively. Taking the superconducting gap to be zero in the F region, and from the Hamiltonian Eq. (1), the excitation energy (relative to the Fermi energy  $E_{FN}$ ) can be obtained as below:



**Fig. 1.** Sketch of the Monolayer Molybdenum disulfide F/S junction with the proximity  $s$ - and  $d$ -wave symmetries. The junction can be a normal/superconductor N/S, when the exchange field  $h$  becomes zero.

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