Transition from T^{-4} to T^{-1} behavior of conductivity and violation of Matthiessen's rule in *p*-type monolayer MoS_2 from acoustic phonon scattering

Xiao-Qin Yu,[1,2,3] Qing-Lian Xu,[2] Zhen-Gang Zhu,[1,2,4,*] and Gang Su[2,4,5,†]

[1]*School of Electronic, Electrical and Communication Engineering, University of Chinese Academy of Sciences, Beijing 100049, China*
[2]*Theoretical Condensed Matter Physics and Computational Materials Physics Laboratory, College of Physical Sciences, University of Chinese Academy of Sciences, Beijing 100049, China*
[3]*School of Physics and Electronics, Hunan University, Changsha 410082, China*
[4]*CAS Center for Excellence in Topological Quantum Computation, University of Chinese Academy of Sciences, Beijing 100190, China*
[5]*Kavli Institute of Theoretical Sciences, University of Chinese Academy of Sciences, Beijing 100049, China*

(Received 25 July 2018; revised manuscript received 11 January 2019; published 4 February 2019)

The electrical transport of *p*-type monolayer MoS_2 from acoustic phonon scattering at low temperature ($T <$ 100 K) is theoretically analyzed. The formalism of conductivity is systemically derived through the standard Green's functions technique (a full quantum-mechanical treatment) by taking into account the realistic band structure of MoS_2. It is found that the main contribution to resistivity is from piezoelectric scattering in the transverse direction. Analogous to graphene, the conductivity exhibits a transition from $\sigma \sim T^{-4}$ temperature dependence in the Bloch-Grüneisen temperature regime to weaker $\sigma \sim T^{-1}$ dependence at high temperature. It is remarkable that we observe the derivation of Matthiessen's rule in the presence of both disorder scattering and phonon scattering due to the abrupt variation of phonon-induced transport scattering rates.

DOI: 10.1103/PhysRevB.99.075404

I. INTRODUCTION

Monolayer MoS_2 and other transition-metal dichalcogenides (TMDCs) represent a new class of two-dimensional materials, intrinsically behaving as semiconductors. Unlike graphene, inversion symmetry is broken in TMDCs, and they exhibit strong spin-orbit coupling (SOC) in the valence band, which leads to a series of spin- and valley-related anomalous transport phenomena for *p*-type TMDCs, such as the spin Hall effect [1], valley Hall effect [1,2], and spin- and valley-related anomalous Nernst effect [3]. The strong SOC and coupling of the spin and valley degrees of freedom in the valence band offer a great chance for spintronics and valleytronics. At present, experiments exploring the spin and valley effect in MoS_2 are usually conducted below 100 K [2,4]. Thus, *p*-type electrical conductivity of TMDCs at finite temperature is highly desired for fundamental understanding of valleytronics and spintronics in these materials.

Unlike the extensive studies on the electrical transport in *n*-type MoS_2 both experimentally [5–7] and theoretically [8–11], few works study the conductivity of *p*-type MoS_2. In our work, *p*-type MoS_2 means that the Fermi level can be tuned into the valence band by a gate voltage. Recently, an electrolytic gate technique [12] was employed in graphene, and high electron (hole) density can be obtained. Impurity and acoustic phonon scattering dominate the scattering at temperature below 100 K, while the optical phonon scattering is usually not activated [11]. Moreover, the impurity scattering can be diminished by dielectric engineering [12]. The conductivity determined by acoustic phonon scattering therefore gives rise to an upper limit of conductivity at low temperature.

In this work, we theoretically study the electrical transport in *p*-type MoS_2 by considering the acoustic phonon scattering. We start from a realistic phonon model derived from the band structure of MoS_2 rather than a simplified model so that we can have results closer to possible experiments. We derive a formalism for conductivity of *p*-type MoS_2 by using the standard Green's function [13–15] based on the Kubo formula at low temperature. The current-vertex correction within the first Born approximation (FBA) is taken into account through the self-consistent process.

II. THEORETICAL DERIVATION

In the presence of the electron-phonon interaction, the effective Hamiltonian of MoS_2 valley τK is given by

$$\hat{H} = \sum_{\tau\mathbf{k}} \Psi^{+}_{\tau\mathbf{k}} \hat{H}^{0}_{\tau\mathbf{k}} \Psi_{\tau\mathbf{k}} + \sum_{\mathbf{q}\iota} \omega_{\mathbf{q}\iota} a^{+}_{\mathbf{q}\iota} a_{\mathbf{q}\iota} + \sum_{\mathbf{kq},\iota\tau\tau'} \Psi^{+}_{\tau\mathbf{k+q}} \hat{g}^{\iota}_{\tau\mathbf{k+q},\tau'\mathbf{k}} \Psi_{\tau'\mathbf{k}} (a_{\mathbf{q}\iota} + a^{+}_{-\mathbf{q}\iota}), \quad (1)$$

where $\Psi^{+}_{\tau\mathbf{k}} = (c^{+}_{\tau\mathbf{k},c,\uparrow}, c^{+}_{\tau\mathbf{k},v,\uparrow}, c^{+}_{\tau\mathbf{k},c,\downarrow} c^{+}_{\tau\mathbf{k},v,\downarrow})$ is the fermion operator, $c^{+}_{\tau\mathbf{k},c,s_z}$ ($c^{+}_{\tau\mathbf{k},v,s_z}$) indicates the creation operators of one electron with momentum $\mathbf{k}$ in the conduction (valence) band with spin $s_z = \pm 1$ at valley τK, $\tau = \pm 1$ represent the valley indices, $a^{+}_{\mathbf{q}\iota}$ is the creation operator of one phonon with momentum $\mathbf{q}$ in the ι branch of the phonon, $\omega_{\mathbf{q},\iota}$ refers to the corresponding frequency, $\hat{g}^{\iota}_{\tau\mathbf{k+q},\tau'\mathbf{k}}$ is the electron-phonon matrix element, and $\hat{H}^{0}_{\tau\mathbf{k}}$ is the noninteracting effective

*zgzhu@ucas.ac.cn
†gsu@ucas.ac.cn

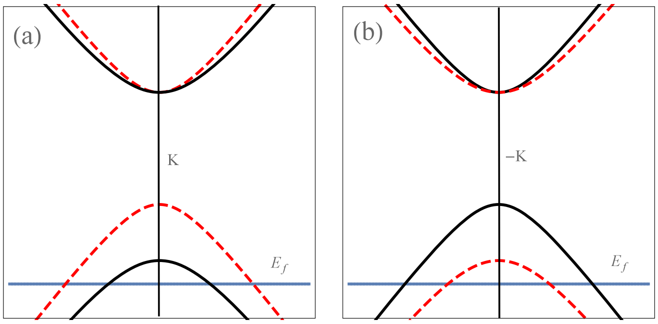

FIG. 1. Schematic of the energy band at valley K ($-K$). Dashed and solid curves indicate the spin-up and spin-down bands, respectively. E_f is the Fermi energy.

Hamiltonian around valley τK and is determined by [1]

$$\hat{H}^0_{\tau\mathbf{k}} = at(\tau k_x\hat{\sigma}_x + k_y\hat{\sigma}_y) + \frac{\Delta}{2}\hat{\sigma}_z + \frac{\lambda\tau}{2}(\hat{\sigma}_z - 1)\hat{s}_z = \begin{pmatrix} \hat{H}^0_{\uparrow\tau\mathbf{k}} & 0 \\ 0 & \hat{H}^0_{\downarrow\tau\mathbf{k}} \end{pmatrix}, \tag{2}$$

with $\hat{H}^0_{s_z\tau\mathbf{k}} = \frac{\Delta'}{2}\hat{\sigma}_z + \frac{s_z\lambda\tau}{2}\hat{\sigma}_I + at\tau k_x\hat{\sigma}_x + atk_y\hat{\sigma}_y$, where 2λ is the spin splitting at the top of the valence band caused by the SOC, $\hat{\sigma}$ denotes the Pauli matrices for the two basis functions of the energy bands, a is the lattice constant, t is the hopping integral, Δ is the energy gap, $\Delta' = \Delta - \lambda$ is the spin-dependent band gap, and $\hat{s}_z$ represents the Pauli matrix for spin. The energy eigenvalues are

$$\varepsilon_{n_0\tau s_z}(k) = s_z\frac{\lambda\tau}{2} + n_0\sqrt{(kat)^2 + \left(\frac{\Delta - s_z\lambda\tau}{2}\right)^2}, \tag{3}$$

where $n_0 = \pm 1$ is the band index. The corresponding band structures are schematically shown for the two valleys in Figs. 1(a) and 1(b). The spin- and valley-coupled band structures are clearly identified.

We here concentrate on the electron-phonon scattering with the acoustic modes at low temperature ($T < 100$ K, $100k_B \approx 8.617$ meV) containing both deformation potential (DP) and piezoelectric (PE) scattering. Kaasbjerg *et al.* [10] showed that the acoustic phonons exist below energy less than 30 meV, while the optical phonons can be excited at 35–60 meV. Moreover, they showed that, in the temperature regime with which we are concerned (<100 K), the scatterings from the intervalley acoustic phonons and optical phonons are strongly suppressed and can be neglected [10]. In addition, due to the strong spin-valley coupling in the valence band, the intervalley scattering is suppressed for the p-type MoS_2 in the absence of atomic-scale magnetic scatters [1]. For simplicity, we assume the acoustic phonon interactions for the electron and hole are identical. Therefore, the coupling strength $\hat{g}^{\iota}_{\tau\mathbf{k+q},\tau'\mathbf{k}}$ behaves as

$$\hat{g}^{\iota}_{\tau\mathbf{k+q},\tau'\mathbf{k}} \approx \hat{g}^{\iota}_{\tau\mathbf{q},\tau'} = \sqrt{\frac{\hbar}{2\rho A\omega_{\mathbf{q}\iota}}}M^{\iota}_{\tau\mathbf{q}}\delta_{\tau,\tau'}\hat{I}, \tag{4}$$

where A is the area of the sample, ρ is the atomic mass density per area, $\hbar$ is Planck's constant, and $M^{\iota}_{\tau\mathbf{q}}$ is the coupling matrix element for the given valley, τK, which is assumed to be independent of the k vector of the carriers [10]. To get Eq. (4), the electron-phonon coupling for intravalley scattering processes is approximated by the electron-phonon coupling at the bottom of the valleys, i.e., $|\mathbf{k}| = 0$, with the momentum located at K, K'. The matrix elements for $\tau = -1$ (namely, $-K$) are related through the time-reversal symmetry as $M^{\iota}_{\tau=-1,\mathbf{q}} = M^{\iota}_{\tau=1,-\mathbf{q}}$. Thus, we will show only the coupling matrix elements $M^{\iota}_{\tau=1,\mathbf{q}}$ of the K valley explicitly, and the coupling matrix elements from the $-K$ valley can be deduced by the time-reversal symmetry. Therefore, it is expressed as $M^{\iota}_{\mathbf{q}}$ in the following.

For acoustic phonon scattering, in the long-wavelength limit [11], both frequency $w_{\mathbf{q},\iota}$ and the coupling matrix element of the transverse-acoustic (TA) and longitudinal-acoustic (LA) modes are linear in q, i.e.,

$$w_{\mathbf{q},\iota} = c_\iota|\mathbf{q}|, \quad \left|M^{\iota}_{\mathbf{q}}\right| = \left(\Xi^{\mathrm{DP}}_{\iota} + \Xi^{\mathrm{PE}}_{\iota}\right)|\mathbf{q}|, \tag{5}$$

where c_ι is the sound velocity, $\Xi^{\mathrm{DP}}_{\iota}$ is the acoustic deformation potential, $\Xi^{\mathrm{PE}}_{\iota} = \frac{1}{\sqrt{2}}(\frac{e_{11}e}{\epsilon_0})$ is the effective isotropic piezoelectric coupling strength, e_{11} is the piezoelectric constant, and ϵ_0 indicates the vacuum permeability. The noninteracting Green's function of MoS_2, in the Matsubara space, is

$$\hat{G}^0_{\tau}(\mathbf{k}, i\omega_n) = \left[(i\omega_n + \mu)\hat{I}_4 - \hat{H}^0_{\tau\mathbf{k}}\right]^{-1} = \begin{pmatrix} \hat{G}^0_{\uparrow\tau}(\mathbf{k}, i\omega_n) & 0 \\ 0 & \hat{G}^0_{\downarrow\tau}(\mathbf{k}, i\omega_n) \end{pmatrix}, \tag{6}$$

where $i\omega_n$ is the Matsubara frequency for fermions and $\hat{G}^0_{s_z\tau}(\mathbf{k}, i\omega_n)$ is the spin-dependent noninteracting Green's function and is given by $\hat{G}^0_{s_z\tau}(\mathbf{k}, i\omega_n) = [(i\omega_n + \mu)\hat{\sigma}_I - \hat{H}^0_{s_z\tau\mathbf{k}}]^{-1}$. We can expand the s_z-spin-dependent Green's function in the Pauli matrix basis, namely, $\hat{G}^0_{s_z\tau}(\mathbf{k}, i\omega_n) = \sum_{j=I,x,y,z}\hat{G}^0_{s_z\tau,j}(\mathbf{k}, i\omega_n)\hat{\sigma}_j$, where $\hat{G}^0_{s_z\tau,I}(\mathbf{k}, i\omega_n) = \hat{G}^0_{s_z\tau,+}(E_{s_z\tau}, i\omega_n)$, $\hat{G}^0_{s_z\tau,x}(\mathbf{k}, i\omega_n) = \gamma_{\mathrm{off}}(E_{s_z\tau})\hat{G}^0_{s_z\tau,-}(E_{s_z\tau}, i\omega_n)\tau\cos\phi$, $\hat{G}^0_{s_z\tau,y}(\mathbf{k}, i\omega_n) = \gamma_{\mathrm{off}}(E_{s_z\tau})\hat{G}^0_{s_z\tau,-}(E_{s_z\tau}, i\omega_n)\sin\phi$, and $\hat{G}^0_{s_z\tau,z}(\mathbf{k}, i\omega_n) = \gamma_{\mathrm{z}}(E_{s_z\tau})\hat{G}^0_{s_z\tau,-}(E_{s_z\tau}, i\omega_n)$, with $\hat{G}^0_{s_z\tau,\pm}(E_{s_z\tau}, i\omega_n) = \frac{1}{2}[g^0_{s_z\tau,+}(E_{s_z\tau}, i\omega_n) \pm g^0_{s_z\tau,-}(E_{s_z\tau}, i\omega_n)]$, where

$$g^0_{s_z\tau,\pm}(E_{s_z\tau}, i\omega_n) = \frac{1}{i\omega_n + \mu - \frac{s_z\tau\lambda}{2} \mp E_{s_z\tau}}, \tag{7}$$

$\gamma_{\mathrm{off}}(E_{s_z\tau}) = \epsilon_1/E_{s_z\tau}$, and $\gamma_{\mathrm{z}}(E_{s_z\tau}) = \Delta'/2E_{s_z\tau}$. We denote $\epsilon_1 = atk$ and $E_{s_z\tau} = \sqrt{(atk)^2 + (\Delta'/2)^2}$. The intrinsically p doped MoS_2 is concerned with $|\mu| \gg \omega_{\max}$ ($\omega_{\max} = 2c_\iota\hbar k_F$ is the allowed exchanged phonon energies induced by the acoustic phonon scattering, and the constraint can be fulfilled in MoS_2 since $v_F \gg c_\iota$), $\mu < 0$, and the electronic states restricted to the Fermi surface: $s_z\tau\lambda/2 - E_{s_z\tau} \approx \mu$ and $\epsilon_1 \approx \sqrt{(s_z\tau\lambda/2 - \mu)^2 - (\Delta'/2)^2}$. In this case, $\gamma_{\mathrm{off}}(E_{s_z\tau})$ is written as $\gamma^{\mathrm{off}}_{s_z\tau} \approx \sqrt{1 - (\Delta')^2/(2\mu - s_z\tau\lambda)^2}$, and $\gamma_{\mathrm{z}}(E_{s_z\tau})$ is reexpressed as $\gamma^{\mathrm{z}}_{s_z\tau} \approx \Delta'/(s_z\tau\lambda - 2\mu)$.

To determine the electrical transport properties, the full Green's function $\hat{G}_\tau(\mathbf{k}, i\omega_n)$ is evaluated through Dyson's equation,

$$\hat{G}_\tau(\mathbf{k}, i\omega_n)^{-1} = \hat{G}^0_\tau(\mathbf{k}, i\omega_n)^{-1} - \hat{\Sigma}^{\mathrm{1BA}}_\tau(\mathbf{k}, i\omega_n), \tag{8}$$

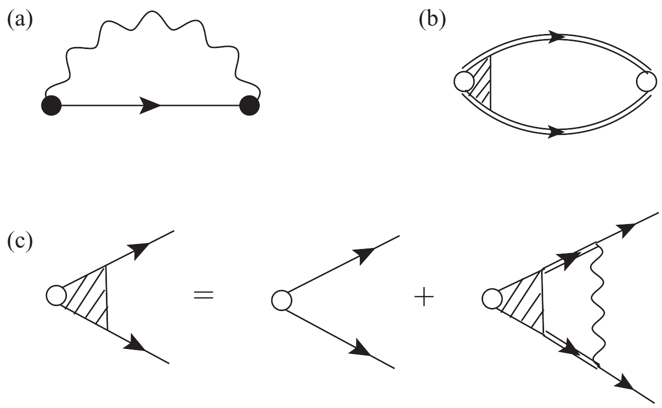

FIG. 2. (a) Illustration of first Born approximation for the self-energy. The single straight solid line represents the noninteraction Green's function, and the wavy line is the phonon propagator. (b) Diagrammatic representation of the current-current response function Π_{xx}. The double straight line indicates the full Green's function, and the open circle is the velocity vertex $\hat{v}_x$. (c) The particle renormalized current vertex $v_{\rm F}\hat{\Gamma}_x$ with phonon insertions.

where $\hat{\Sigma}^{1\rm BA}_{\tau}(\mathbf{k}, i\omega_n)$ is the self-energy determined through the FBA [Fig. 2(a)] and has the following form:

$$\Sigma^{1\rm BA}_{\tau}(\mathbf{k}, i\omega_n) = \frac{-1}{\beta A}\sum_{ip_n,\mathbf{k}'\iota}\left|\hat{g}^{\iota}_{\mathbf{k}-\mathbf{k}'}\right|^2 D^0_{\iota}(\mathbf{k}-\mathbf{k}', ip_n - i\omega_n) \times \hat{G}^0_{\tau}(\mathbf{k}', ip_n), \tag{9}$$

where ip_n are Matsubara frequencies for fermions, $D^0_{\iota}(\mathbf{q}, iq_n) = \frac{1}{iq_n-\omega_{\mathbf{q},\iota}} - \frac{1}{iq_n+\omega_{\mathbf{q},\iota}}$ is the free-equilibrium-phonon Green's function, where iq_n is the Matsubara frequency for bosons. Owing to the spin independence of the electron-phonon coupling $\hat{g}^{\iota}_{\mathbf{k}-\mathbf{k}'}$ and the free-phonon Green's function, the self-energy $\Sigma^{1\rm BA}_{\tau}(\mathbf{k}, i\omega_n)$ is also diagonal in spin space. Replacing the free Green's function $\hat{G}^0_{\tau}$ by the spin-dependent Green's function $\hat{G}^0_{s_z\tau}$ in Eq. (9), one can obtain the formula of spin-dependent self-energy, which can be further decomposed into the Pauli matrix as

$$\hat{\Sigma}^{1\rm BA}_{s_z\tau}(\mathbf{k}, i\omega_n) = \sum_{j=I,x,y,z}\Sigma^{1\rm BA}_{s_z\tau,j}(\mathbf{k}, i\omega_n)\hat{\sigma}_j, \tag{10}$$

where $\Sigma^{1\rm BA}_{s_z\tau,j=I,z}(\mathbf{k}, i\omega_n) = \Sigma^{1\rm BA}_{s_z\tau,j=I,z}(E_{s_z\tau}, i\omega_n)$, $\Sigma^{1\rm BA}_{s_z\tau,x}(\mathbf{k}, i\omega_n) = \tau\Sigma^{1\rm BA}_{s_z\tau,\rm off}(E_{s_z\tau}, \phi, i\omega_n)\cos\phi$, and $\Sigma^{1\rm BA}_{s_z\tau,y}(\mathbf{k}, i\omega_n) = \Sigma^{1\rm BA}_{s_z\tau,\rm off}(E_{s_z\tau}, \phi, i\omega_n)\sin\phi$. The relevant electron momenta are here restricted to the Fermi surface, i.e., $\mathbf{k}\approx\mathbf{k}_F$ [$\varepsilon_{s_z\tau}(k)=\mu$], so that the self-energy depends only on the angular part of the $\mathbf{k}$ vector, giving $\Sigma^{1\rm BA}_{s_z\tau,j}(E_{s_z\tau}, \phi, i\omega_n) \to \Sigma^{1\rm BA}_{s_z\tau,j}(\phi, i\omega_n)$. The sum over $\mathbf{k}'$ can be split into its energy and angular integrals: $\sum_{\mathbf{k}'} \to \int_{-\pi}^{\pi}\frac{d\phi}{2\pi}\int d\varepsilon N_{s_z\tau}(\varepsilon)$ [here, $\varepsilon = \frac{s_z\tau\lambda}{2} - \sqrt{(atk)^2 + (\Delta'/2)^2}$], where $N_{s_z\tau}(\varepsilon) = \frac{A}{2\pi}\frac{|\varepsilon - s_z\tau\lambda/2|}{a^2t^2}$ is the density of states for spin s_z and valley τ. It is noted that $N_{s_z\tau}(\varepsilon) = 0$ when the energy ε lies in the gap. Thus, we have

$$\Sigma^{1\rm BA}_{s_z\tau,j}(\phi, i\omega_n) = \frac{-1}{\beta}\sum_{\iota,i\omega_m}\int_0^{2\pi}\frac{d\phi'}{2\pi}\gamma_j(\phi')G^{0,\rm loc}_{s_z\tau,j}(i\omega_m) \times\int d\Omega\frac{2\Omega\alpha^2F_{\iota}(\phi-\phi',\Omega)}{\Omega^2-(i\omega_n-i\omega_m)^2}, \tag{11}$$

where $\beta = 1/k_{\rm B}T$; $\gamma_{j=I,z}(\phi')=1$; $\gamma_x(\phi')=\tau\cos\phi'$; $\gamma_y(\phi')=\sin\phi'$; $G^{0,\rm loc}_{s_z\tau,j}(i\omega_m)$ indicates the local ($\mathbf{k}$-averaged) Green's function, $G^{0,\rm loc}_{s_z\tau,I}(i\omega_m)\approx N_{s_z\tau}(\mu)\int dE_{s_z\tau}G^0_{s_z\tau,+}(E_{s_z\tau}, i\omega_m)$ and $G^{0,\rm loc}_{s_z\tau,j=x,y,z}(i\omega_m)\approx N_{s_z\tau}(\mu)\int dE_{s_z\tau}G^0_{s_z\tau,-}(E_{s_z\tau}, i\omega_m)$; and $\alpha^2F_{\iota}(\phi-\phi',\Omega)$ is the Eliashberg function introduced via $\alpha^2F_{\iota}(\mathbf{k}-\mathbf{k}',\Omega) = |g^{\iota}_{\mathbf{k}-\mathbf{k}'}|^2\delta(\Omega-\omega_{\mathbf{k}-\mathbf{k}',\iota})$. Decomposing Eq. (11) in the spherical harmonics basis (see Appendix A), one can get the diagonal and off-diagonal components of the self-energy in Eq. (11) as

$$\Sigma^{1\rm BA}_{s_z\tau,I}(i\omega_n) = \frac{1}{\beta}\sum_{m,\iota}\int d\Omega\frac{2\Omega\alpha^2F_{\iota,0}(\Omega)}{\Omega^2-(i\omega_n-i\omega_m)^2}G^{0,\rm loc}_{s_z\tau,+}, \tag{12}$$

$$\Sigma^{1\rm BA}_{s_z\tau,z}(i\omega_n) = \frac{\gamma^z_{s_z\tau}}{\beta}\sum_{m,\iota}\int d\Omega\frac{2\Omega\alpha^2F_{\iota,0}(\Omega)}{\Omega^2-(i\omega_n-i\omega_m)^2}G^{0,\rm loc}_{s_z\tau,-}, \tag{13}$$

$$\Sigma^{1\rm BA}_{s_z\tau,\rm off}(i\omega_n) = \frac{\gamma^{\rm off}_{s_z\tau}}{\beta}\sum_{m,\iota}\int d\Omega\frac{2\Omega\alpha^2F_{\iota,1}(\Omega)}{\Omega^2-(i\omega_n-i\omega_m)^2}G^{0,\rm loc}_{s_z\tau,-}, \tag{14}$$

where $G^{0,\rm loc}_{s_z\tau,\pm} = G^{0,\rm loc}_{s_z\tau,\pm}(i\omega_m)$ and $\alpha^2F_{\iota,v}$ are the projection of the Eliashberg function $\alpha^2F_{\iota}(\phi)$ on the spherical Harmonics with $v = 0, \pm1, \pm2, \ldots$. The retarded self-energy $\Sigma^{1\rm BA}_{s_z\tau,j=0,\rm off,z}(\omega+i\eta)$ can easily be obtained by taking the analytical continuation ($i\omega_n\to\omega+i\eta$ with $\eta\to0^+$) of Eqs. (12)–(14) on the real-frequency axis using standard techniques. According to the imaginary part of the retarded self-energy, we thus define the frequency-dependent scattering rate $\Gamma^{j=0,\rm off,z}_{s_z\tau}(\omega) = -{\rm Im}\Sigma^{1\rm BA}_{s_z\tau,j=0,\rm off,z}(\omega+i\eta)$. The scattering rates are given (see also Appendix B) by

$$\Gamma^I_{s_z\tau}(\omega) = K^0_{s_z\tau}(\omega), \quad \Gamma^{\rm off(z)}_{s_z\tau}(\omega) = -\gamma^{\rm off(z)}_{s_z\tau}K^{1(0)}_{s_z\tau}(\omega), \tag{15}$$

with $K^v_{s_z\tau}(\omega) = \sum_{\iota}K^{\iota,v}_{s_z\tau}(\omega)$,

$$K^{\iota,v}_{s_z\tau}(\omega) = \frac{\pi N_{s_z\tau}}{2}(\mu)\sum_{j=\pm1}\int d\Omega\alpha^2F_{\iota,v}(\Omega) \times[n_{\rm B}(\omega)+n_{\rm F}(\Omega+j\omega)]\Theta(\xi), \tag{16}$$

where $\xi = -\mu-\omega-j\Omega-\frac{\Delta-2s_z\tau\lambda}{2}$, $\Theta(\xi)$ is a step function, and $n_{\rm B}$ ($n_{\rm F}$) is the Fermi (Bose) distribution function. For the states at the Fermi energy, which involve only the lower band ($\mu<0$), the total quasiparticle scattering rate can be defined as

$$\Gamma^{\rm pq}_{s_z\tau}(\omega) = \Gamma^0_{s_z\tau}(\omega) - \left[\gamma^{\rm off}_{s_z\tau}\Gamma^{\rm off}_{s_z\tau}(\omega) + \gamma^z_{s_z\tau}\Gamma^z_{s_z\tau}(\omega)\right] = \sum_{\iota}\left\{\left[1+\left(\gamma^z_{s_z\tau}\right)^2\right]K^{\iota,0}_{s_z\tau}(\omega) + \left(\gamma^{\rm off}_{s_z\tau}\right)^2K^{\iota,1}_{s_z\tau}(\omega)\right\}. \tag{17}$$

With the help of the Dyson equation in Eq. (8) and some careful derivations described in Appendix A, one can determine the full retarded Green's function taking into account the acoustic electron-phonon interaction in the analogous form of the noninteracting Matsubara Green's function matrix, with $i\omega_n\to\omega+i\eta$ and replacing the undressed Green's function in Eq. (7) by

$$g_{s_z\tau,\pm}(E_{s_z\tau}, \omega+i\eta) = \frac{1}{\omega+\mu-\frac{s_z\tau\lambda}{2}\mp E_{s_z\tau}+i\Gamma^{\rm pq}_{s_z\tau}}. \tag{18}$$

Taking the conjugate to the retarded Green's function, the advanced Green's function $\hat{G}(E_{s_z\tau}, \omega-i\eta)$ can be determined.

According to the Kubo formalism, the imaginary-time current-current correlation function $\Pi^{11}_{j,j'}$ is defined as

$$\Pi^{11}_{j,j'}(\tau_t) = \frac{1}{V}\langle T_\tau J_j(\tau_t) J_{j'}(0)\rangle, \tag{19}$$

where $J_j(\tau_t) = \sum_{\mathbf{k}} \Psi^+_{\mathbf{k}}(\tau_t) \upsilon_j \Psi_{\mathbf{k}}(\tau_t)$ is the j component of the particle current; υ_j is the j component of the velocity, which is given by $\hbar\vec{v}_{\mathbf{k}} = at(\tau\hat{\sigma}_x \vec{e}_{k_x} \otimes \hat{s}_I + \hat{\sigma}_y \vec{e}_{k_y} \otimes \hat{s}_I)$; and τ_t indicates the imaginary time. In terms of the definition of $J_j(\tau_t)$ and the conserving approximation consistent with the FBA of the single-particle Green's function, Π^{11}_{xx} [Fig. 2(b)] in the frequency space can be obtained as

$$\begin{aligned}\Pi^{11}_{xx}(i\omega_n) &= \frac{a^2t^2}{A\beta\hbar^2} \sum_{\mathbf{k} s_z\tau, i\omega_m} \mathrm{Tr}\big[\tau\hat{\sigma}_x \hat{G}_{s_z\tau}(\mathbf{k}, i\omega_m) \\ &\quad \times \hat{\Gamma}^x_{s_z\tau}(\mathbf{k}, i\omega_m, i\omega_n + i\omega_m)\hat{G}_{s_z\tau}(\mathbf{k}, i\omega_n + i\omega_m)\big] \\ &= \frac{1}{\beta}\sum_{i\omega_m} P_{xx}(i\omega_m, i\omega_n + i\omega_m),\end{aligned} \tag{20}$$

where the dimensionless vertex function $\hat{\Gamma}^x_{s_z\tau}$ can be evaluated within the self-consistent ladder approximation [Fig. 2(c)]

$$\begin{aligned}\hat{\Gamma}^x_{s_z\tau}(\mathbf{k}, n, n+m) &= \tau\hat{\sigma}_x + \frac{1}{A\beta}\sum_{\mathbf{k}', l, \iota}\big[|\hat{g}_{\mathbf{k}-\mathbf{k}',\iota}|^2 D^0_\iota \\ &\quad \times (\mathbf{k}-\mathbf{k}', n-l)\hat{G}_{s_z\tau}(\mathbf{k}', l)\hat{\Gamma}^x_{s_z\tau} \\ &\quad \times (\mathbf{k}', l, l+m)\hat{G}_{s_z\tau}(\mathbf{k}', l+m)\big].\end{aligned} \tag{21}$$

For simplicity, l, n, m are used to represent $i\omega_l, i\omega_n, i\omega_m$, respectively. Considering only low-energy scattering caused by electron-phonon interaction and the analogous approximation in self-energy, for the vertex function, one can have $|\mathbf{k}| \approx k_F$ and retain only the angular dependence, namely, $\hat{\Gamma}^x_{s_z\tau}(\mathbf{k}, i\omega_1, i\omega_2) \approx \hat{\Gamma}^x_{s_z\tau}(\phi, i\omega_1, i\omega_2)$. In addition, the vertex function can be decomposed in the basis of the Pauli matrices as

$$\hat{\Gamma}^x_{s_z\tau}(\phi, i\omega_1, i\omega_2) = \sum_{j=I,x,y,z} y_{s_z\tau,j}(\phi, i\omega_1, i\omega_2)\hat{\sigma}_j. \tag{22}$$

With the properties of Pauli matrices, we have

$$y_{s_z\tau,j}(\phi, i\omega_1, i\omega_2) = \tfrac{1}{4}\mathrm{Tr}\big\{\hat{\sigma}_j, \hat{\Gamma}^x_{s_z\tau}(\phi, i\omega_1, i\omega_2)\big\}. \tag{23}$$

Expanding $y_{s_z\tau,j}(\phi, i\omega_1, i\omega_2)$ in terms of the spherical harmonics components, $y_{s_z\tau,j}(\phi, i\omega_1, i\omega_2) = \sum_v y_{s_z\tau,j}(i\omega_1, i\omega_2)e^{iv\phi}$. After a series of careful derivations described in Appendix C, the longitudinal conductivity can be written as

$$\begin{aligned}\sigma_{xx} &= \frac{e^2a^2t^2}{\hbar A}\sum_{s_z\tau}\int_{-\infty}^{\infty}\frac{d\omega'}{2\pi}\left(-\frac{dn_{\rm F}(\omega')}{d\omega'}\right)\tau\big\{y^{\rm AR,tot}_{s_z\tau}(\omega',\omega') \\ &\quad \times b^{\rm AR}_{s_z\tau}(\omega',\omega') - \mathrm{Re}\big[y^{\rm RR,tot}_{s_z\tau}(\omega',\omega')b^{\rm RR}_{s_z\tau}(\omega',\omega')\big]\big\},\end{aligned} \tag{24}$$

where $b^{\rm XY}_{s_z\tau}(\omega',\omega') = N_{s_z\tau}(\mu)\int dE_{s_z\tau} G^{\rm X}_{s_z\tau,+}G^{\rm Y}_{s_z\tau,+}$ and $b^{\rm AR}_{s_z\tau}(\omega',\omega') \approx N_{s_z\tau}(\mu)/4\Gamma^{\rm pq}_{s_z\tau}(\omega')$, X and Y represent retarded (R) or advanced (A), and $y^{\rm XY,tot}_{s_z\tau}(\omega',\omega') = \sum_{vj} c^v_j y^{v,\rm XY}_{s_z\tau,j}(\omega',\omega')$, where $y^{v,\rm XY}_{s_z\tau,j}(\omega',\omega')$ is the analytic continuation of $y^v_{s_z\tau,j}(i\omega_1, i\omega_2)$, with $y^{v,\rm RR}_{s_z\tau,j}(\omega',\omega') = y^v_{s_z\tau,j}(\omega'+i\eta, \omega'+i\eta)$ and $y^{v,\rm AR}_{s_z\tau,j}(\omega',\omega') = y^v_{s_z\tau,j}(\omega'-i\eta, \omega'+i\eta)$. The coefficients c^v_j are numerical coefficients which arise from the angular average over ϕ and are given in Eq. (C20). $y^{\rm RR,tot}_{s_z\tau}(\omega',\omega')$ can be determined via the Ward identity [13] (see Appendix C) as

$$y^{\rm RR,tot}_{s_z\tau}(\omega',\omega') = \tau\big(\chi^{\rm off}_{s_z\tau}\big)^2\left(1 - i\frac{\Gamma^{\rm off}_{s_z\tau}(\omega')}{\hbar v_{\rm F}k_F}\right). \tag{25}$$

Here, $y^{\rm AR,tot}_{s_z\tau}(\omega',\omega')$ can be solved through a single self-consistent equation with the solution (see Appendix C)

$$\begin{aligned}y^{v,\rm AR}_{s_z\tau,I}(\omega') &= \frac{K^v_{s_z\tau}(\omega')}{2\Gamma^{\rm pq}_{s_z\tau}(\omega')}\sum_{j\beta} h^\beta_j y^{v+\beta,\rm AR}_{s_z\tau,j}(\omega'), \\ y^{v,\rm AR}_{s_z\tau,x}(\omega') &= \delta_{v,0} + \frac{K^v_{s_z\tau}(\omega')}{2\Gamma^{\rm pq}_{s_z\tau}(\omega')}\sum_{j\beta} c^\beta_j y^{v+\beta,\rm AR}_{s_z\tau,j}(\omega'), \\ y^{v,\rm AR}_{s_z\tau,y}(\omega') &= \frac{K^v_{s_z\tau}(\omega')}{2\Gamma^{\rm pq}_{s_z\tau}(\omega')}\sum_{j\beta} d^\beta_j y^{v+\beta,\rm AR}_{s_z\tau,j}(\omega'), \\ y^{v,\rm AR}_{s_z\tau,z}(\omega') &= \frac{K^v_{s_z\tau}(\omega')}{2\Gamma^{\rm pq}_{s_z\tau}(\omega')}\sum_{j\beta} f^\beta_j y^{v+\beta,\rm AR}_{s_z\tau,j}(\omega'),\end{aligned} \tag{26}$$

where the expansion coefficients are given in Eq. (C20). By exploiting the symmetric/antisymmetric properties of $v \to -v$ of the $I, x, y,$ and z components, it can be found that there are only four nonzero independent components: $y^{1,\rm AR}_{s_z\tau,I}(\omega')$, $y^{1,\rm AR}_{s_z\tau,z}(\omega')$, $y^{0,\rm AR}_{s_z\tau,x}(\omega')$, and $y^{2,\rm AR}_{s_z\tau,x}(\omega')$ with the relations $y^{2,\rm AR}_{s_z\tau,x}(\omega') = y^{-2,\rm AR}_{s_z\tau,x}(\omega') = i\tau y^{2,\rm AR}_{s_z\tau,y}(\omega') = -i\tau y^{-2,\rm AR}_{s_z\tau,y}(\omega')$, $y^{1,\rm AR}_{s_z\tau,I}(\omega') = y^{-1,\rm AR}_{s_z\tau,I}(\omega')$, and $y^{1,\rm AR}_{s_z\tau,z}(\omega') = y^{-1,\rm AR}_{s_z\tau,z}(\omega')$. Putting these relations into Eq. (26) and the definition of $y^{\rm AR,tot}_{s_z\tau}(\omega',\omega')$ yields

$$y^{\rm AR,tot}_{s_z\tau}(\omega') = \frac{2\tau\big(\chi^{\rm off}_{s_z\tau}\big)^2\Gamma^{\rm pq}_{s_z\tau}(\omega')}{\Gamma^{\rm tr}_{s_z\tau}(\omega')}, \tag{27}$$

where the energy-dependent transport scattering rate $\Gamma^{\rm tr}_{s_z\tau}(\omega') = \sum_\iota \Gamma^{\rm tr,\iota}_{s_z\tau}(\omega')$ is given by

$$\begin{aligned}\Gamma^{\rm tr,\iota}_{s_z\tau}(\omega') &= \big(\gamma^{\rm off}_{s_z\tau}\big)^{-2}\big\{\big[2\big(\gamma^{\rm off}_{s_z\tau}\big)^2\big]K^{\iota,0}_{s_z\tau}(\omega') - 2\big(\gamma^z_{s_z\tau}\big)^2 K^{\iota,1}_{s_z\tau}(\omega') \\ &\quad - \big(\gamma^{\rm off}_{s_z\tau}\big)^2 K^{\iota,2}_{s_z\tau}(\omega')\big\}.\end{aligned} \tag{28}$$

Substituting Eq. (27) into Eq. (24) and neglecting the insignificant second term [13], the conductivity is now simplified as

$$\sigma_{\rm tot} = \frac{e^2a^2t^2}{\hbar A}\sum_{s_z\tau}\int_{-\infty}^{\infty}\frac{d\omega'}{2\pi}\left(\frac{-dn_{\rm F}(\omega')}{d\omega'}\right)\frac{N_{s_z\tau}(\mu)}{\sum_\iota \Gamma^{\rm tr,\iota}_{s_z\tau}(\omega')}. \tag{29}$$

III. RESULTS AND DISCUSSION

$\Gamma^{\rm tr,\iota}_{s_z\tau} = \Gamma^{\rm tr,\iota}_{s_z\tau}(\omega' = 0)$ depends on temperature for different values of $s_z\tau$ and phonon modes, as shown in Figs. 3(a) and 3(b). In the low-temperature regime $T \ll T_{\rm BG}$, where $T_{\rm BG} = 2\hbar v_\iota k_{\rm F}/k_{\rm B}$ is the Bloch-Grüneisen temperature [11,12,16], the transport scattering rates behave as $\Gamma^{\rm tr,\iota}_{s_z\tau} \approx T^4$ (refer to Appendix A). In the limit of high temperature, $T \gg T_{\rm BG}$, the transport scattering rate $\Gamma^{\rm tr}_{s_z\tau}$, as expected, varies linearly with T. In this temperature regime, the number of phonons linearly

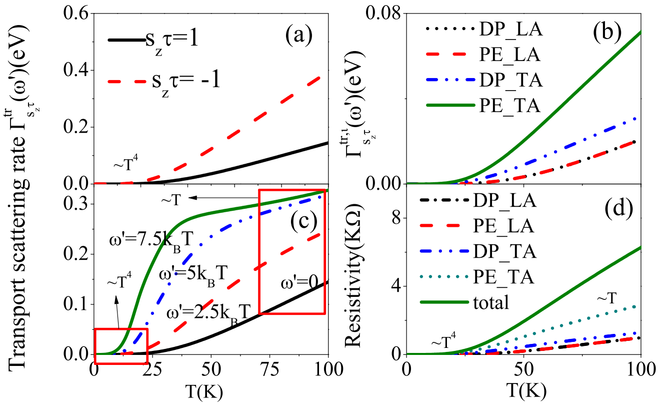

FIG. 3. The transport scattering rates $\Gamma(\omega')$ are calculated as a function of temperature for different values of (a) $s_z\tau$, (b) phonon modes, and (c) energy ω'. The energy ω' in (a) and (c) is taken at 0 eV. $s_z\tau = 1$ is fixed in (b) and (c). The phonon mode in (a) and (c) is chosen to be the transverse mode of acoustic deformation. (d) The temperature dependence of the resistivity of MoS_2. Here, $E_f = -1.1$ eV, and all material parameters are given in Table I.

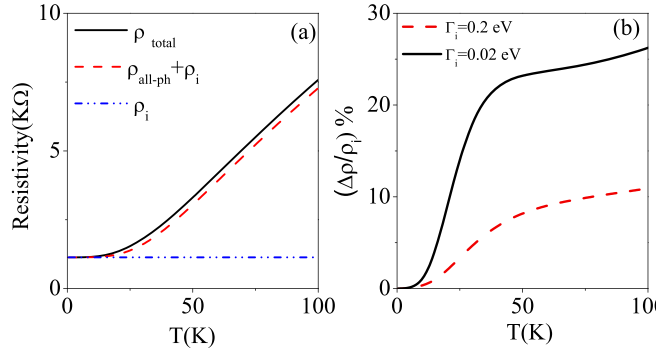

FIG. 4. The deviations from Matthiessen's rule. Here, $\rho_{\rm i}$ and $\rho_{\text{all-ph}}$ are the resistivities induced by impurities and phonons, respectively. The subscript "all" in $\rho_{\text{all-ph}}$ indicates that all four phonon modes (DP_LA, PE_LA, DP_TA, and PE_TA) are included. (b) The ratio of the deviation in the resistivity to ρ_i as a function of temperature for different impurity scattering rates $\Gamma_i = 0.2$ and 0.02 eV, where $\Delta\rho = \rho_{\rm total} - (\rho_{\text{all-ph}} + \rho_i)$. In (a), $\Gamma_i = 0.02$ eV. Here, $E_f = -1.1$ eV, and all material parameters are given in Table I.

depends on temperature ($n_B \approx k_{\rm B}T/\hbar\omega$), leading to the linear temperature dependence of $K^{\iota,v}_{s_z\tau}(\omega) = 2N_{s_z\tau}(\mu)\zeta_v I_\iota k_{\rm B}T/\hbar c_\iota$ in Eq. (28), where the coefficient ζ_v is given in Eq. (A11). We observe that the impact of transverse modes on the transport scattering rate is stronger than those of the longitudinal modes, and the transverse mode due to the effective isotropic piezoelectric interaction is dominant [Fig. 3(b)]. Therefore, the low-temperature resistivity ($1/\sigma_{\rm total}$) for pure p-type MoS_2 is mainly contributed by the transverse piezoelectric scattering [Fig. 3(d)]. The piezoelectric coupling to acoustic phonons results from the lack of an inversion center of the MoS_2 crystal.

Figure 3(c) shows the variation of the transport scattering rate $\Gamma^{\rm tr}_{s_z\tau}(\omega')$ with temperature at different ω'. Two limits can be observed. At low-temperature limit, the transport scattering rates show a T^4 dependence, while they exhibit a linear T dependence at the high-temperature limit. This gives rise to a transition from a low-temperature Bloch-Grüneisen regime resistivity $\rho \sim T^4$ behavior to a weaker $\rho \sim T$ at high temperature. It is also seen that the transport scattering rate is sensitively energy dependent. With increasing ω', it rises faster and more abruptly at low temperature, while it tends to a saturation value at high temperature for larger ω'.

The effect of disorder manifests itself through a phenomenological method [13,17] in which the imaginary part of the self-energy, i.e., $\Gamma_i = \hbar/\tau_i$ (where τ_i is the average lifetime of the quasiparticle), is introduced into the full Matsubara Green's function [Eq. (18)], namely, $\Gamma^{\rm pq}(\omega') \to \Gamma^{\rm pq}(\omega') + \Gamma_i$. This replacement can provide us the correct and qualitative results for the impurity scattering. The impurity-induced resistivity ρ_i in the absence of phonon scattering is independent of the temperature, as expected (see Fig. 4). However, the total resistivity $\rho_{\rm total} = 1/\sigma_{\rm total}$ induced by both phonons and impurities at low temperature is no longer T^4 dependent; $\sigma_{\rm total}$ is given in Eq. (30), in which the effects of the acoustic phonon scattering and impurity scattering are taken into account already. It is observed from Fig. 4 that $\rho_{\rm total}$ is not equal to $\rho_{\rm i} + \rho_{\text{all-ph}}$, which means that Matthiessen's rule (MR) is not fulfilled. The deviation from Matthiessen's rule has been studied systematically for alloys experimentally [18,19] and theoretically [19–21]. Here, the deviation from MR may be attributed to the abrupt variation of the phonon-induced transport scattering rate $\Gamma^{{\rm tr},\iota}_{s_z\tau}(\omega')$ [Fig. 3(c)] for ω' towards the vicinity of the zero point, i.e., $\omega' = 0$ (namely, the Fermi level). At low temperature, the ratio of deviation in the resistivity ($\Delta\rho/\rho_i$) is close to zero, while it rises quickly and abruptly with persistently increasing temperature but gradually grows slower at high temperature [Fig. 4(b)]. This behavior of deviation in the resistivity is essentially consistent with that of $\Gamma^{{\rm tr},\iota}_{s_z\tau}(\omega')|_{\omega'=7.5k_{\rm B}T,5k_{\rm B}T,\ldots} - \Gamma^{{\rm tr},\iota}_{s_z\tau}(0)$ versus T [Fig. 3(c)], indicating that the deviation might result from the variation of the phonon-induced transport scattering rate towards energy ω'. The ratio $\Delta\rho/\rho_i$ is suppressed with increasing scattering strength [see $\Gamma_i = 0.2$ eV in Fig. 4(b)], which is consistent with previous studies of the Cu-Au alloy [19]. The temperature at which the deviation appears in MoS_2 is lower than that in graphene (refer to the third paper in Ref. [16]). This might be due to the lower Bloch-Grüneisen temperature in MoS_2-type materials, which is about $11\sqrt{n}$ for the transverse acoustic phonon, where n is the carrier density, and $18\sqrt{n}$ for the longitudinal acoustic phonon [11]; it is higher in graphene, i.e., $54\sqrt{n}$. Another reason might be the sensitive dependence of the deviation on the disorder level that is different from that of graphene.

Analogous to the derivation of Eq. (29), the total longitudinal conductivity including the phonon and impurity scattering now has the form

$$\sigma_{\rm total} \approx -\frac{(eat)^2}{\hbar V}\sum_{s_z\tau}\int_{-\infty}^{\infty}\frac{d\omega'}{2\pi}\frac{n'_F N_{s_z\tau}(\mu)}{\sum_\iota \Gamma^{{\rm tr},\iota}_{s_z\tau}(\omega') + \Gamma_i}, \qquad (30)$$

where $n'_F = (\frac{dn_{\rm F}(\omega')}{d\omega'})$ develops a peak at $\omega' = 0$ and is essentially zero when the energy is beyond the range of $[-10k_BT, 10k_BT]$. The functions $\Gamma^{{\rm tr},\iota}_{s_z\tau}(\omega')$ vary rapidly in this region. Thus, the denominator in the last term of Eq. (30), i.e., $\sum_\iota \Gamma^{\mathrm{tr},\iota}_{s_z\tau}(\omega') + \Gamma_i$, cannot be taken out of the integration. The total resistivity ρ_{total} thus cannot be divided into two independent parts (namely, $1/\sigma_{\text{all-ph}}$ and $1/\sigma_{\mathrm{i}}$). Even for almost constant $\Gamma^{\mathrm{tr},\iota}_{s_z\tau}(\omega')$, the equality $1/\sigma_{\mathrm{total}} = 1/\sigma_{\text{all-ph}} + 1/\sigma_{\mathrm{i}}$ is not satisfied owing to the summation on spins.

IV. CONCLUSION

In summary, we studied the electrical behavior of p-type MoS_2 constrained by acoustic phonon scattering at low temperature through the standard Feynman diagram technique based on the MoS_2-specified electron-phonon interaction. We found that the main contribution to resistivity is the piezoelectric scattering of the transverse mode of phonons. The resistivity exhibits a $\rho \sim T^4$ temperature dependence in the Bloch-Grüneisen temperature regime and a weaker $\rho \sim T$ dependence at relatively high temperature. It is remarkable that we observe the derivation of Matthiessen's rule when further considering the disorder scattering owing to the abrupt variation of the phonon-induced transport scattering rate.

ACKNOWLEDGMENTS

This work is supported by the Hundred Talents Program of the Chinese Academy of Sciences and the NSFC (Grant No. 11674317). G.S. is supported in part by the MOST (Grant No. 2018FYA0305800), the NSFC (Grants No. 11474279 and No. 11834014), and the CAS (Grant No. XDB07010100). This work is supported in part by the Strategic Priority Research Program of the Chinese Academy of Sciences (Grant No. XDB28000000). X.-Q.Y. is also supported by the Fundamental Research Funds for the Central Universities from China.

APPENDIX A: SPHERICAL HARMONICS EXPANSION

The spherical harmonics expansion $\psi_v(\phi)$ is defined as

$$\psi_v(\phi) = e^{iv\phi}, \quad v = 0, \pm 1, \pm 2, \ldots. \tag{A1}$$

Any generic angle-dependent function $S(\phi)$ can be decomposed on this basis as

$$S(\phi) = \sum_v S_v \psi_v(\phi), \quad S_v = \int_0^{2\pi} \frac{d\phi}{2\pi} S(\phi)\psi_v^*(\phi). \tag{A2}$$

The angle-dependent component of Eq. (11) can be written in the form

$$C_{n'}(\phi) = \int_0^{2\pi} \frac{d\phi'}{2\pi} \mathrm{A}(\phi - \phi')\mathrm{B}(\phi')e^{in'\phi'}. \tag{A3}$$

The Harmonic component C_v of function $C(\phi)$ is

$$\begin{aligned} C_v &= \int_0^{2\pi} \frac{d\phi}{2\pi} e^{-iv\phi} \int_0^{2\pi} \frac{d\phi'}{2\pi} A(\phi - \phi')B(\phi')e^{in'\phi'} \\ &= \int_0^{2\pi}\int_0^{2\pi} \frac{d\phi}{2\pi}\frac{d\phi'}{2\pi} e^{in'\phi'} e^{-iv\phi} \sum_{n,m} A_n e^{in(\phi-\phi')} B_m e^{im\phi'} \\ &= \sum_{n,m} \int_0^{2\pi} \frac{d\phi}{2\pi} e^{-i(v-n)\phi} \int_0^{2\pi} \frac{d\phi'}{2\pi} e^{i(n'+m-n)\phi'} A_n B_m \\ &= \sum_m \delta_{m,v-n'} A_v B_m. \end{aligned} \tag{A4}$$

To obtain Eq. (A4), we have used the property $\int_0^{2\pi} \frac{d\phi}{2\pi} \psi_v^*(\phi) = \delta_{v,0}$.

The explicit expressions for the harmonic components of the Eliashberg function $\alpha^2 F_{\iota,v}(\omega)$ and $K^{\iota,v}_{s_z\tau}(\omega)$ coefficient will be derived. The momentum-dependent Eliashberg function is defined as

$$\alpha^2 F_\iota(\mathbf{k} - \mathbf{k}', \Omega) = \left|g^\iota_{\mathbf{k}-\mathbf{k}'}\right|^2 \delta(\Omega - \omega_{\mathbf{k}-\mathbf{k}',\iota}), \tag{A5}$$

where $g^\iota_{\mathbf{q}} = g^\iota_{\tau\mathbf{q},\tau}$ is given in Eq. (4). As mentioned in the main text, electron momenta are constrained on the Fermi surface: $|\mathbf{k}| \approx |\mathbf{k}'| \approx k_{\mathrm{F}}$, giving $|\mathbf{q}| = 2k_{\mathrm{F}} \sin[(\phi - \phi')/2]$. The Eliashberg function thus depends on only the exchange angle $\phi - \phi'$, namely,

$$\begin{aligned} \alpha^2 F_\iota(\phi - \phi', \Omega) &= 2I_\iota k_F \sin\left[\frac{\phi - \phi'}{2}\right] \\ &\quad \times \delta\left[\Omega - \omega_{\max} \sin\left(\frac{\phi - \phi'}{2}\right)\right], \end{aligned} \tag{A6}$$

where $I_\iota = \hbar \Xi_\iota^2/(2\rho A c_\iota)$. Hence,

$$\begin{aligned} \alpha^2 F_{\iota,v}(\omega) &= 2I_\iota k_F \int_0^{2\pi} \frac{d(\phi - \phi')}{2\pi} \sin\left(\frac{\phi - \phi'}{2}\right) \\ &\quad \times e^{iv(\phi-\phi')} \delta\left[\Omega - \omega_{\max} \sin\left(\frac{\phi - \phi'}{2}\right)\right] \\ &= 2I_\iota k_F \int_0^{\pi} \frac{d\theta}{\pi} \sin\theta e^{2iv\theta} \delta(\Omega - \omega_{\max}\sin\theta). \end{aligned} \tag{A7}$$

To obtain the second line, we have made the variable transformation, i.e., $(\phi - \phi')/2 \to \theta$. The δ function has two solutions for $\theta \in [0, \pi]$: one for $\theta = y_\Omega$ and another for $\theta = \pi - y_\Omega$ with $y_\Omega = \arcsin \frac{\Omega}{\omega_{\max}}$. Therefore, we reach

$$\begin{aligned} \alpha^2 F_{\iota,v}(\omega) &= 2I_\iota k_F \int_0^{\pi} \frac{d\theta}{\pi} \sin\theta e^{2iv\theta} \frac{1}{|\omega_{\max}\cos\theta|} \\ &\quad \times [\delta(\theta - y_\Omega) + \delta(\theta - \pi + y_\Omega)] \\ &= \frac{2I_\iota}{\pi\hbar c_\iota} \frac{\Omega\theta(\omega_{\max} - \Omega)\cos(2vy_\Omega)}{\sqrt{\omega_{\max}^2 - \Omega^2}}, \end{aligned} \tag{A8}$$

where we used the relations $\sin(y_\Omega) = \sin(\pi - y_\Omega) = \frac{\Omega}{\omega_{\max}}$ and $|\cos y_\Omega| = |\cos(\pi - y_\Omega)| = \sqrt{1 - \frac{\Omega^2}{\omega_{\max}^2}}$. $\omega_{\max} = 2\hbar c_\iota k_{\mathrm{F}}$ is the highest exchanged phonon energy [14]. Owing to $\cos(-2vy_\Omega) = \cos(2vy_\Omega)$, we have $\alpha^2 F_{\iota,-v}(\omega) = \alpha^2 F_{\iota,v}(\omega)$. Substituting Eq. (A8) into Eq. (16), we have

$$\begin{aligned} K^{\iota,v}_{s_z\tau}(\omega) &= \frac{N_{s_z\tau}(\mu)I_\iota}{\hbar c_\iota} \sum_j \int_0^{\omega_{\max}} \frac{\theta(\xi)\Omega d\Omega}{\sqrt{\omega_{\max}^2 - \Omega^2}} \\ &\quad \times \cos\left(2v \arcsin\frac{\Omega}{\omega_{\max}}\right)[n_{\mathrm{B}}(\Omega) + n_{\mathrm{F}}(\Omega + j\omega)], \end{aligned} \tag{A9}$$

where $\xi = -\mu - \omega - j\Omega - (\Delta - 2s_z\tau\lambda)/2$. In the relatively high temperature limit $k_{\mathrm{B}}T \gg \omega_{\max}$, the following result occurs: $n_B(\Omega) \approx k_{\mathrm{B}}T/\hbar\Omega \gg 1$, giving rise to

$$K^{\iota,v}_{s_z\tau}(\omega) \approx \frac{2N_{s_z\tau}(\mu)\zeta_v I_\iota}{\hbar c_\iota} k_{\mathrm{B}}T, \tag{A10}$$

where

$$\zeta_v = \int_0^{\omega_{\max}} \frac{\theta(\xi)d\Omega}{\hbar\sqrt{\omega_{\max}^2 - \Omega^2}} \cos\left(2v \arcsin\frac{\Omega}{\omega_{\max}}\right). \quad (A11)$$

We will study the property of $K^{\iota,v}_{s_z\tau}(0)$ at the low-temperature limit $T \ll \omega_{\max}$. When modulating the Fermi energy in the regime where the Fermi energy is sufficiently below the top of the valence band, i.e., $-\mu - (\Delta - 2s_z\tau\lambda)/2 > \omega_{\max}$, the highest exchanged phonon energy $\omega_{\max}$ caused by the acoustic phonon scattering in MoS_2 is smaller than 30 meV [10], and the step function $\theta(\xi)$ will be identically equal to 1. Let $x = \beta\Omega$ in Eq. (A9); we have

$$K^{\iota,v}_{s_z\tau}(0) = \frac{2N_{s_z\tau}(\mu)I_\iota}{\hbar c_\iota}\frac{1}{\omega_{\max}\beta^2}\int_0^{\beta\omega_{\max}} \frac{xdx}{\sqrt{1-(x/\beta\omega_{\max})^2}} \times \cos\left(2v\arcsin\frac{x}{\beta\omega_{\max}}\right)[n_B(x)+n_F(x)]. \quad (A12)$$

In the limit of low temperature $T \ll \omega_{\max}$, only the leading terms in powers of $y/\beta\omega_{\max}$ in the integrand will be retained, and the upper limit of integration can be expanded to infinity, i.e., $\beta\omega_{\max} \to \infty$, giving rise to

$$K^{\iota,v}_{s_z\tau}(0) = \frac{2N_{s_z\tau}(\mu)I_\iota}{\hbar c_\iota}\frac{k_B^2T^2}{\omega_{\max}}\left(b_1 + b_3\frac{1-4v^2}{2}\frac{k_B^2T^2}{\omega_{\max}^2}\right), \quad (A13)$$

where $b_n = \int_0^\infty dx x^n[n_B(x) + f_B(x)]$, with the solutions $b_1 = \pi^2/4$ and $b_3 = \pi^4/8$. Substituting Eq. (A13) into the expression for $\Gamma^{\text{tr},\iota}_{s_z\tau}(0)$ [Eq. (28)], the transport scattering rate $\Gamma^{\text{tr},\iota}_{s_z\tau}$ at $\omega' = 0$ is found,

$$\Gamma^{\text{tr},\iota}_{s_z\tau}(0) = \frac{2N_{s_z\tau}(\mu)I_\iota\pi^4}{8\hbar c_\iota}\frac{4+4(\gamma^{\text{off}}_{s_z\tau})^2}{(\gamma^{\text{off}}_{s_z\tau})^2}\frac{k_B^4T^4}{\omega_{\max}^3}. \quad (A14)$$

To obtain the above equation, we have applied the relation $(\gamma^{\text{off}}_{s_z\tau})^2 + (\gamma^z_{s_z\tau})^2 = 1$.

APPENDIX B: THE SCATTERING RATE $\Gamma^j_{s_z\tau}(\omega)$ AND FULL RETARDED GREEN'S FUNCTION MATRIX $\hat{G}_{s_z\tau}(\mathbf{k}, i\omega_n)$

The Matsubara sums that have to be evaluated in Eqs. (12)–(14) can all be written in the form

$$A_\pm(i\omega_n) = \frac{1}{\beta}\sum_{i\omega_m}\frac{2\Omega}{\Omega^2 - (i\omega_n - i\omega_m)^2}G^{0,\text{loc}}_{s_z\tau,\pm}(i\omega_m). \quad (B1)$$

The sum over fermionic frequencies $i\omega_m$ in Eq. (B1) can be converted into

$$\begin{aligned} A_\pm(i\omega_n) = {} & [n_B(\Omega)+1]G^{0,\text{loc}}_{s_z\tau,\pm}(i\omega_n - \Omega) + n_B(\Omega)G^{0,\text{loc}}_{s_z\tau,\pm} \\ & \times(i\omega_n + \Omega) + \frac{N_{s_z\tau}(\mu)}{2}\int_{\frac{\Delta'}{2}}^\infty dE_{s_z\tau}n_F \\ & \times\left(E_{s_z\tau} + \frac{s_z\tau\lambda}{2} - \mu\right)\left[g^0_{s_z\tau,+}(E_{s_z\tau}, i\omega_n + \Omega)\right. \\ & \left.- g^0_{s_z\tau,+}(E_{s_z\tau}, i\omega_n - \Omega)\right] \pm \frac{N_{s_z\tau}(\mu)}{2}\int_{\frac{\Delta'}{2}}^\infty dE_{s_z\tau}n_F \\ & \times\left(-E_{s_z\tau} + \frac{s_z\tau\lambda}{2} - \mu\right)\left[g^0_{s_z\tau,-}(E_{s_z\tau}, i\omega_n + \Omega)\right. \\ & \left.- g^0_{s_z\tau,-}(E_{s_z\tau}, i\omega_n - \Omega)\right], \end{aligned} \quad (B2)$$

with

$$G^{0,\text{loc}}_{s_z\tau,\pm}(i\omega_n) = \tfrac{1}{2}\left[g^{0,\text{loc}}_{s_z\tau,+}(i\omega_n) \pm g^{0,\text{loc}}_{s_z\tau,-}(i\omega_n)\right] \quad (B3)$$

and $g^{0,\text{loc}}_{s_z\tau,\pm}(i\omega_n) = N_{s_z\tau}(\mu)\int dE_{s_z\tau}g^0_{s_z\tau,\pm}(E_{s_z\tau}, i\omega_n)$, where $g^0_{s_z\tau,\pm}(E_{s_z\tau}, i\omega_n)$ is given in Eq. (7). As mentioned in the main text, we focus on the properties of p-type MoS_2, which means $\mu < 0$. Taking the analytical continuation $i\omega_n \to \omega + i\eta$ $(\eta \to 0^+)$, one finds the imaginary part of $A_\pm(\omega + i\eta)$ to be

$$\text{Im}A_\pm(\omega + i\eta) = \mp\frac{\pi N_{s_z\tau}(\mu)}{2}\sum_{j=\pm1}[n_B(\omega) + n_F(\Omega + j\omega)] \times\Theta\left(-\mu - j\Omega - \frac{\Delta + 2s_z\tau\lambda}{2} - \omega\right). \quad (B4)$$

In order to obtain Eq. (B4), we use the equality $\text{Im}\int_{\frac{\Delta'}{2}}^\infty dE_{s_z\tau}\frac{1}{a+E_{s_z\tau}+i\eta} = \Theta(-a - \frac{\Delta'}{2})$. Based on Eqs. (12), (13), (14), (B2), and (B4), we obtain the formula of frequency-dependent scattering rates $\Gamma^{j=0,\text{off},z}_{s_z\tau}(\omega) = -\text{Im}\Sigma^{1\text{BA}}_{s_z\tau,j}(\omega + i\eta)$ shown in Eq. (15).

The real part of phonon self-energy is nearly zero and can be neglected, and the spin-dependent retarded self-energy matrix can thus be approximately written as

$$\hat{\Sigma}^{1\text{BA}}_{s_z\tau}(\omega + i\eta) = -\sum_{j=0,z} i\gamma_j(\phi)\Gamma^j_{s_z\tau}(\omega)\hat{\sigma}_j - \sum_{j=x,y} i\gamma_j(\phi)\Gamma^{\text{off}}_{s_z\tau}(\omega)\hat{\sigma}_j, \quad (B5)$$

with $\gamma_{j=0,z}(\phi) = 1$, $\gamma_x(\phi) = \tau\cos\phi$, and $\gamma_y(\phi) = \sin\phi$. Substituting Eq. (B5) into the spin-dependent Dyson equation, analogous to Eq. (8) except replacing subscript τ by $s_z\tau$, the spin-dependent full retarded Green's function is found to be

$$\hat{G}^R_{s_z\tau}(E_{s_z\tau}, \omega)^{-1} = \left(\omega + \mu - \frac{s_z\tau\lambda}{2} + i\Gamma^0_{s_z\tau}\right)\hat{\sigma}_I + \left(i\Gamma^z_{s_z\tau} - \frac{\Delta'}{2}\right)\hat{\sigma}_z + \left(i\Gamma^{\text{off}}_{s_z\tau} - \epsilon_1\right)(\tau\cos\phi\hat{\sigma}_x + \sin\phi\hat{\sigma}_y), \quad (B6)$$

where $\epsilon_1 = atk = \sqrt{E^2_{s_z\tau} - \frac{(\Delta')^2}{4}}$. The spin-dependent full retarded Green's function can be expanded in the Pauli matrix as

$$\hat{G}^R_{s_z\tau}(E_{s_z\tau}, \omega) = \sum_{j=I,x,y,z}\hat{G}^R_{s_z\tau,j}(E_{s_z\tau}, \omega)\hat{\sigma}_j, \quad (B7)$$

with

$$\hat{G}^R_{s_z\tau,I}(E_{s_z\tau}, \omega) = \frac{1}{2}(g_{s_z\tau,+} + g_{s_z\tau,-}),$$

$$\hat{G}^R_{s_z\tau,j}(E_{s_z\tau}, \omega) = \frac{1}{2}(g_{s_z\tau,+} - g_{s_z\tau,-})\vec{F}_j, \quad j = x, y, z,$$

$$\vec{F} = \frac{(c\tau\cos\phi, c\sin\phi, \frac{\Delta'}{2} - i\Gamma^z_{s_z\tau})}{\sqrt{c^2 + (\frac{\Delta'}{2} - i\Gamma^z_{s_z\tau})^2}},$$

$$g_{s_z\tau,\pm} = \frac{1}{\omega + \mu - E'_{s_z\tau,\pm}(E_{s_z\tau}, \omega)},$$

$$E'^{,\mathrm{R}}_{s_z\tau,\pm}(E_{s_z\tau},\omega)=\frac{s_z\lambda\tau}{2}+\Gamma^0_{s_z\tau}\pm\sqrt{c^2+\left(\frac{\Delta'}{2}-i\Gamma^z_{s_z\tau}\right)^2},$$
$$c=\left(\epsilon_1-i\Gamma^{\mathrm{off}}_{s_z\tau}\right).\tag{B8}$$

In order to identify the total effective quasiparticle scattering rate, we expand the square-root part of the energy band $E'^{,\mathrm{R}}_{s_z\tau,\pm}(E_{s_z\tau},\omega)$ in Eq. (B8),

$$c^2+\left(\frac{\Delta'}{2}-i\Gamma^z_{s_z\tau}\right)^2={\epsilon_1}^2+\left(\frac{\Delta'}{2}\right)^2-2i\left(\epsilon_1\Gamma^{\mathrm{off}}_{s_z\tau}+\frac{\Delta'}{2}\Gamma^z_{s_z\tau}\right)-\left(\Gamma^z_{s_z\tau}\right)^2-\left(\Gamma^{\mathrm{off}}_{s_z\tau}\right)^2.\tag{B9}$$

Since ${\epsilon_1}^2+(\frac{\Delta'}{2})^2=E^2_{s_z\tau}=(\mu-\frac{s_z\tau\lambda}{2})^2\approx\mu^2$ and $\Gamma^0_{s_z\tau}$, $\Gamma^{\mathrm{off}}_{s_z\tau}$, $\Gamma^z_{s_z\tau}\ll|\mu|$, we can neglect the second order of $\Gamma^j_{s_z\tau}$, and at the same order, we have

$$\begin{aligned}&{\epsilon_1}^2+\left(\frac{\Delta'}{2}\right)^2-2i\left(\epsilon_1\Gamma^{\mathrm{off}}_{s_z\tau}+\frac{\Delta'}{2}\Gamma_z\right)\\&\approx\left[E_{s_z\tau}-i\left(\sqrt{1-\left(\frac{\Delta'}{2E_{s_z\tau}}\right)^2}\Gamma^{\mathrm{off}}_{s_z\tau}+\frac{\Delta'}{2E_{s_z\tau}}\Gamma^z_{s_z\tau}\right)\right]^2\\&\approx\left[E_{s_z\tau}-i\left(\gamma_{\mathrm{off}}\Gamma^{\mathrm{off}}_{s_z\tau}+\gamma_z\Gamma^z_{s_z\tau}\right)\right]^2.\end{aligned}\tag{B10}$$

Thus, the modified energy band is found to be

$$E'^{,\mathrm{R}}_{s_z\tau,\pm}(E_{s_z\tau},\omega)=\frac{s_z\lambda\tau}{2}\pm E_{s_z\tau}-i\Gamma^{\pm}_{s_z\tau},\tag{B11}$$

where the $+$ $(-)$ in $\pm$ refers to the conduction (valence) band and $\Gamma^{\pm}_{s_z\tau}$ is the quasiparticle scattering rate given by

$$\Gamma^{\pm}_{s_z\tau}=\Gamma^0_{s_z\tau}\pm\left(\gamma^{\mathrm{off}}_{s_z\tau}\Gamma^{\mathrm{off}}_{s_z\tau}+\gamma^z_{s_z\tau}\Gamma^z_{s_z\tau}\right).\tag{B12}$$

Putting the expression for $E'^{,\mathrm{R}}_{s_z\tau,\pm}(E_{s_z\tau},\omega)$ in Eq. (B11) into Eq. (B8), we can determine the full retarded Green's function. In addition, by changing $\Gamma^j_{s_z\tau}\longrightarrow-\Gamma^j_{s_z\tau}$ in Eqs. (B6) and (B8), the advanced full Green's function $\hat{G}_{s_z\tau}(E_{s_z\tau},\omega-i\eta)$ can be determined.

APPENDIX C: EXPRESSION OF CONDUCTIVITY σ_{xx} IN THE PRESENCE OF ACOUSTIC PHONON SCATTERING

In this appendix, the expression for conductivity [Eq. (24)] will be derived in detail. The sum over fermion frequencies $i\omega_m$ in Eq. (20) can be converted to an integral,

$$\begin{aligned}\Pi^{11}_{xx}(i\omega_n)=\frac{-1}{2\pi i}\int_{-\infty}^{\infty}d\omega' n_{\mathrm{F}}(\omega')[&P_{xx}(\omega'+i\eta,\omega'+i\omega_n)\\&-P_{xx}(\omega'-i\eta,\omega'+i\omega_n)+P_{xx}(\omega'-i\omega_n,\omega'+i\eta)\\&-P_{xx}(\omega'-i\omega_n,\omega'-i\eta)].\end{aligned}\tag{C1}$$

Analytical continuation $i\omega_n\to\omega+i\eta$ and variable change $\omega'\to\omega'+\omega$ in the last two terms bring us to the result

$$\begin{aligned}\Pi^{11}_{xx}(\omega+i\eta)=\int_{-\infty}^{\infty}\frac{d\omega'}{2\pi i}\{&[n_{\mathrm{F}}(\omega')-n_{\mathrm{F}}(\omega'+\omega)]\\&\times P^{\mathrm{AR}}_{xx}(\omega',\omega'+\omega)-n_{\mathrm{F}}(\omega')P^{\mathrm{RR}}_{xx}(\omega',\omega'+\omega)\\&+n_{\mathrm{F}}(\omega'+\omega)P^{\mathrm{AA}}_{xx}(\omega',\omega'+\omega)\}.\end{aligned}\tag{C2}$$

The longitudinal conductivity σ_{xx} in the Kubo formula is given by

$$\sigma_{xx}=-\lim_{\omega\to0}\frac{e^2}{\omega}\mathrm{Im}\,\Pi^{11}_{xx}(\omega+i\eta).\tag{C3}$$

Here, we should notice that $\hbar\omega$ has been written as ω in $\Pi^{11}_{xx}(\omega+i\eta)$. So the next step is to take the limit $\omega\to0$ in Eq. (C2). Based on the relation $P_{xx}(z_1,z_2)=P_{xx}(z_2,z_1)$, $P^{\mathrm{AR}}_{xx}(\omega',\omega')=P_{xx}(\omega'-i\eta,\omega'+i\eta)$ is real. And $P^{RR}_{xx}(\omega',\omega'+\omega)=P_{xx}(\omega'+i\eta,\omega'+\omega+i\eta)$ is the complex conjugate of $P^{AA}_{xx}(\omega',\omega'+\omega)=P_{xx}(\omega'-i\eta,\omega'+\omega-i\eta)$. Thus, we derive

$$\sigma_{xx}=\int_{-\infty}^{\infty}\frac{\hbar d\omega'}{2\pi}(-n'_F)\left[P^{\mathrm{AR}}_{xx}(\omega',\omega')-\mathrm{Re}P^{\mathrm{RR}}_{xx}(\omega',\omega')\right].\tag{C4}$$

Substituting Eq. (22) into Eq. (20), we obtain

$$\begin{aligned}P_{xx}(m,n+m)=\frac{\tau a^2t^2}{A\hbar^2}\sum_{\mathbf{k}s_z\tau j}&L_{s_z\tau,1j}(\mathbf{k},m,n+m)\\&\times y_{s_z\tau,j}(\mathbf{k},m,n+m),\end{aligned}\tag{C5}$$

with

$$L_{s_z\tau,1j}(\mathbf{k},m,n+m)=\mathrm{Tr}\left[\tau\hat{\sigma}_x\hat{G}_{s_z\tau}(\mathbf{k},m)\hat{\sigma}_j\hat{G}_{s_z\tau}(\mathbf{k},n+m)\right],\tag{C6}$$

where l,n, and m denote $i\omega_l$, $i\omega_n$, and $i\omega_m$ for simplicity, respectively. Similar to the self-energy, the relevant electron momenta are assumed to be constrained on the Fermi surface, i.e., $|\mathbf{k}|\approx|\mathbf{k}'|\approx k_{\mathrm{F}}$, $\mathbf{k}\to(k_{\mathrm{F}},\phi)$, and $\sum_{\mathbf{k}}\to N_{s_z\tau}(\mu)\int\frac{d\phi}{2\pi}\int d\varepsilon_{s_z\tau}$. With the relation $\varepsilon_{s_z\tau}=s_z\tau\lambda/2-E_{s_z\tau}$ (for the hole), the integration over $\varepsilon_{s_z\tau}$ can be changed into $E_{s_z\tau}$. Meanwhile, expanding the ϕ-dependent part, i.e., $\int_0^{2\pi}\frac{d\phi}{2\pi}L_{s_z\tau,1j}(\phi)y_{s_z\tau,j}(\phi)$ in terms of spherical harmonics (Appendix A), we obtain

$$P_{xx}(m,n+m)=\frac{\tau a^2t^2}{A\hbar^2}\sum_{vs_zj}c^v_jb_{s_z\tau}(m,n+m)y^v_{s_z\tau,j}(m,n+m),\tag{C7}$$

with

$$\begin{aligned}b_{s_z\tau}(m,n+m)=N_{s_z\tau}(\mu)\int_{\frac{\Delta'}{2}}^{\infty}&dE_{s_z\tau}G_{s_z\tau,+}(E_{s_z\tau},m)\\&\times G_{s_z\tau,+}(E_{s_z\tau},n+m).\end{aligned}\tag{C8}$$

The expansion coefficients c^v_j are given in Eq. (C20). Taking the analytical continuation of Eq. (C7), the longitudinal conductivity in Eq. (C4) can be written as

$$\sigma_{xx}=\frac{e^2a^2t^2\tau}{\hbar A}\sum_s\int_{-\infty}^{\infty}\frac{d\omega'}{2\pi}\left(-\frac{dn_{\mathrm{F}}(\omega')}{d\omega'}\right)\sigma_{xx}(\omega'),\tag{C9}$$

with

$$\begin{aligned}\sigma_{xx}(\omega')=y^{\mathrm{AR,tot}}_{s_z\tau}(\omega',\omega')b^{\mathrm{AR}}_{s_z\tau}(\omega',\omega')\\-\mathrm{Re}\left[y^{\mathrm{RR,tot}}_{s_z\tau}(\omega',\omega')b^{\mathrm{RR}}_{s_z\tau}(\omega',\omega')\right],\end{aligned}\tag{C10}$$

where $y^{\mathrm{xx}',\mathrm{tot}}_{s_z\tau}(\omega',\omega')=\sum_{vj}c^v_j y^{v,\mathrm{xx}'}_{s_z\tau,j}(\omega',\omega')$, the superscripts x and x′ refer to retarded (R) or advanced (A), the expansion coefficients c^v_j are given in Eq. (C20), and $y^{v,\mathrm{RR}}_{s_z\tau,j}(\omega',\omega')$ can be determined from the Ward identity [13]:

$$\hat{\Gamma}^{\mathrm{RR}}_{s_z\tau,x}(\mathbf{k},\omega',\omega')=\tau\hat{\sigma}_x+\frac{\partial}{\hbar v_F\partial k_x}\hat{\Sigma}^{\mathrm{1BA}}_{s_z\tau}(\mathbf{k},\omega'+i\eta),\quad \text{(C11)}$$

where $\hat{\Sigma}^{\mathrm{1BA}}_{s_z\tau}(\mathbf{k},\omega'+i\eta)\approx\hat{\Sigma}^{\mathrm{1BA}}_{s_z\tau}(\phi,\omega'+i\eta)$ is given in Eq. (B5), which yields

$$\hat{\Gamma}^{\phi,\mathrm{RR}}_{s_z\tau,x}(\omega',\omega')=\tau\hat{\sigma}_x-i\frac{\Gamma^{\mathrm{off}}_{s_z\tau}(\omega')}{\hbar v_F k_F}\tau\hat{\sigma}_x.\quad \text{(C12)}$$

Here, $v_\mathrm{F}k_\mathrm{F}$ can be determined by the chemical potential

$$\hbar v_\mathrm{F}k_\mathrm{F}=\sqrt{\left(\mu+\frac{\Delta-2s_z\tau\lambda}{2}\right)\left(\mu-\frac{\Delta}{2}\right)}.\quad \text{(C13)}$$

From Eqs. (23) and (C12), we obtain

$$y^{\mathrm{RR}}_{s_z\tau,x}(\omega',\omega')=\tau\left(1-i\frac{\Gamma^{\mathrm{off}}_{s_z\tau}(\omega')}{v_\mathrm{F}k_F}\right),$$
$$y^{\mathrm{RR}}_{s_z\tau,I}(\omega',\omega')=y^{\mathrm{RR}}_{s_z\tau,y}(\omega',\omega')=y^{\mathrm{RR}}_{s_z\tau,z}(\omega',\omega')=0.\quad \text{(C14)}$$

Here, we can find that $y^{\mathrm{RR}}_{s_z\tau,j}(\omega',\omega')$ is independent of ϕ. Based on the properties of spherical harmonics expansion, only $y^{0,\mathrm{RR}}_{s_z\tau,j}(\omega',\omega')=y^{\mathrm{RR}}_{s_z\tau,j}(\omega',\omega')$ is nonzero. Therefore,

$$y^{\mathrm{RR,tot}}_{s_z\tau}=c^0_x y^{0,\mathrm{RR}}_{s_z\tau,x}(\omega',\omega')=\tau\chi^2_{\mathrm{off}}\left(1-i\frac{\Gamma^{\mathrm{off}}_{s_z\tau}(\omega')}{\hbar v_\mathrm{F}k_\mathrm{F}}\right).\quad \text{(C15)}$$

In the following, we will deduce the solution of $y^{v,\mathrm{AR}}_{s_z\tau,j}(\omega')$. Owing to the constraint (i.e., $|\mathbf{k}|\approx k_\mathrm{F}$), the $\mathbf{k}$-dependent function depends on the directional angle ϕ of the momentum, and the summation over $\mathbf{k}'$ can be converted into $\sum_{\mathbf{k}'}\to N_{s_z\tau}(\mu)\int\frac{d\phi}{2\pi}\int dE_{s_z\tau}$. Therefore, the dimensionless current vertex momentum-dependent $\hat{\Gamma}^x_{s_z\tau}(\mathbf{k},n,n+m)\approx\hat{\Gamma}^x_{s_z\tau}(\phi,n,n+m)$ in Eq. (21) within the self-consistent ladder approximation can be rewritten as

$$\hat{\Gamma}^x_{s_z\tau}(\phi,n,n+m)=\tau\sigma_x+\frac{N_{s_z\tau}(\mu)}{\beta V}\sum_{l,\iota}\int_0^{2\pi}\frac{d\phi'}{2\pi}\int dE_{s_z\tau}W_{\phi-\phi',\iota}(n-l)\hat{G}_{s_z\tau}(E_{s_z\tau},l)\hat{\Gamma}^x_{s_z\tau}(\phi',l,l+m)\hat{G}_{s_z\tau}(E_{s_z\tau},l+m),\quad \text{(C16)}$$

where $W_{\phi-\phi',\iota}(n-l)=|\hat{g}_{\phi-\phi',\iota}|^2D^0_\iota(\phi-\phi',n-l)$. For $\mu<0$, the spin-dependent full Green's function matrix is

$$\hat{G}_{s_z\tau}(\mathbf{k},i\omega_n)=\hat{G}_{s_z\tau}(E_{s_z\tau},\phi,i\omega_n)=\tfrac{1}{2}g_{s_z\tau,-}(E_{s_z\tau},i\omega_n)\left[\hat{\sigma}_I-\chi^z_{s_z\tau}\hat{\sigma}_z-\chi^{\mathrm{off}}_{s_z\tau}(\tau\cos\phi\hat{\sigma}_x+\sin\phi\hat{\sigma}_y)\right].\quad \text{(C17)}$$

Substituting Eq. (C16) into Eq. (23), the function $y_{s_z\tau,j}(\phi,n,m)$ is found to be

$$y_{s_z\tau,j}(\phi,n,n+m)=\delta_{1j}+\frac{N_{s_z\tau}(\mu)k_BT}{2}\sum_{j'\iota l}\int_0^{2\pi}\frac{d\phi'}{2\pi}\int dE_{s_z\tau}W_{\phi-\phi',\iota}(n-l)L_{s_z\tau,jj'}(\phi',E_{s_z\tau},l,l+m)y_{s_z\tau,j'}(\phi',l,l+m).\quad \text{(C18)}$$

The matrix $\hat{L}_{s_z\tau}(\phi,E_{s_z\tau},l,l+m)$ is

$$\hat{L}_{s_z\tau}(\phi,E_{s_z\tau},l,l+m)=G_{s_z\tau,+}(E_{s_z\tau},l)G_{s_z\tau,+}(E_{s_z\tau},l+m)\times\begin{pmatrix}4 & -4\tau\chi^{\mathrm{off}}_{s_z\tau}\cos\phi & -4\chi^{\mathrm{off}}_{s_z\tau}\sin\phi & -4\chi^z_{s_z\tau}\\ -4\tau\chi^{\mathrm{off}}_{s_z\tau}\cos\phi & 2(\chi^{\mathrm{off}}_{s_z\tau})^2(1+\cos2\phi) & 2\tau(\chi^{\mathrm{off}}_{s_z\tau})^2\sin2\phi & 4\tau\chi^z_{s_z\tau}\chi^{\mathrm{off}}_{s_z\tau}\cos\phi\\ -4\chi^{\mathrm{off}}_{s_z\tau}\sin\phi & 2\tau(\chi^{\mathrm{off}}_{s_z\tau})^2\sin2\phi & 2(\chi^{\mathrm{off}}_{s_z\tau})^2(1-\cos2\phi) & 4\chi^z_{s_z\tau}\chi^{\mathrm{off}}_{s_z\tau}\sin\phi\\ -4\chi^z_{s_z\tau} & 4\tau\chi^z_{s_z\tau}\chi^{\mathrm{off}}_{s_z\tau}\cos\phi & 4\chi^z_{s_z\tau}\chi^{\mathrm{off}}_{s_z\tau}\sin\phi & 4(\chi^z_{s_z\tau})^2\end{pmatrix}.\quad \text{(C19)}$$

Decomposing $y_{s_z\tau,j}(\phi,i\omega_1,i\omega_2)$ in terms of the spherical harmonics as $\sum_v y^v_{s_z\tau,j}(i\omega_1,i\omega_2)e^{iv\phi}$ and using the standard procedures for the analytical continuation to each element on the right-hand side of Eq. (C18), the coefficients $y^{v,\mathrm{AR}}_{s_z\tau,j}(\omega',\omega')=y^v_{s_z\tau,j}(\omega'-i\eta,\omega'+i\eta)$ are found to have the simple set of algebraic relations given in Eq. (26). The related expansion coefficients are

$$\begin{cases} h_I^0 = 2, \\ \tau h_x^{-1} = \tau h_x^1 = -\chi_{s_z\tau}^{\text{off}}, \\ h_y^{-1} = -h_y^1 = i\chi_{s_z\tau}^{\text{off}}, \\ h_z^0 = -2\chi_{s_z\tau}^z, \\ \text{else } h_j^v = 0, \end{cases} \quad \begin{cases} f_I^0 = -2\chi_{s_z\tau}^z, \\ \tau f_x^{-1} = \tau f_x^1 = \chi_{s_z\tau}^{\text{off}}\chi_{s_z\tau}^z, \\ f_y^{-1} = -f_y^1 = -i\chi_{s_z\tau}^{\text{off}}\chi_{s_z\tau}^z, \\ f_z^0 = 2(\chi_{s_z\tau}^z)^2, \\ \text{else } f_j^v = 0, \end{cases}$$

$$\begin{cases} c_I^{-1} = c_I^1 = -\chi_{s_z\tau}^{\text{off}}, \\ \tau c_x^0 = 1 - (\chi_{s_z\tau}^z)^2, \\ \tau c_x^{-2} = \tau c_x^2 = \frac{(\chi_{s_z\tau}^{\text{off}})^2}{2}, \\ c_y^{-2} = -c_y^2 = -i\frac{(\chi_{s_z\tau}^{\text{off}})^2}{2}, \\ c_z^1 = c_z^{-1} = \chi_{s_z\tau}^z\chi_{s_z\tau}^{\text{off}}, \\ \text{else } c_j^v = 0, \end{cases} \quad \begin{cases} d_I^{-1} = -d_I^1 = i\chi_{s_z\tau}^{\text{off}}, \\ \tau d_x^{-2} = -\tau d_x^2 = -i\frac{(\chi_{s_z\tau}^{\text{off}})^2}{2}, \\ d_y^0 = 1 - (\chi_{s_z\tau}^z)^2, \\ d_y^{-2} = d_y^2 = -\frac{(\chi_{s_z\tau}^{\text{off}})^2}{2}, \\ d_z^{-1} = -d_z^1 = -i\chi_{s_z\tau}^z\chi_{s_z\tau}^{\text{off}}, \\ \text{else } d_j^v = 0, \end{cases} \tag{C20}$$

where $\chi_{s_z\tau}^{\text{off}} \approx \gamma_{s_z\tau}^{\text{off}} \approx \sqrt{1-(\Delta')^2/(2\mu - s_z\tau\lambda)^2}$ and $\chi_{s_z\tau}^z \approx \gamma_{s_z\tau}^z \approx \Delta'/(s_z\lambda\tau - 2\mu)$.

APPENDIX D: SOME DISCUSSION OF THE DISORDER EFFECT

The disorder scattering is another important scattering mechanism which should be studied in more detail. There may be a few types of disorder, including impurities, defects, substituting atoms, etc. Moreover, the specified band structures for the host materials must be considered. From the theoretical aspect, in metals, the effect of disorder scattering is usually treated after averaging over the disorder configurations, restoring the momentum conservation [13,17]. Therefore, this kind of scattering does not induce intervalley transitions which need momentum transfer. A single impurity may induce momentum-transferred scattering if it possesses an intrinsic degree of freedom. For the disorder in MoS_2-type materials, there are studies about the effect of atomic defects on the intervalley scattering in the conduction bands. In addition to the spin-valley coupling, it is shown that the symmetry and positions of atomic defects give rise to unconventional selection rules for intervalley quasiparticle scattering [22]. Because the band structure of valence bands is different from that of conduction bands, the disorder-induced scattering also possesses different characters. Xiao *et al.* [1] showed that spin and valley degrees are coupled, leading to the splitting of the bands for different spins in one valley; that is, the valley-contrasting spin splitting is 0.1–0.5 eV. The spin and valley relaxations are suppressed at the valence-band edges by this splitting. Valley and spin can be simultaneously flipped only in energy conservation processes, which requires atomic-scale magnetic scatters. Therefore, it is reasonable to ignore the intervalley scattering from usual disorders.

TABLE I. Material parameters for MoS_2 used in this work. Apart from the first four parameters, which are taken from Ref. [1], all the parameters are adopted from Ref. [11].

Parameter	Symbol	Value
Lattice constant	a	3.193 Å
Hopping	t	1.1 eV
Spin splitting	2λ	0.15 eV
Energy gap	Δ	1.66 eV
Ion mass density	ρ	3.1×10^{-7} g/cm^2
Effective electron mass	$m^\star$	0.48 m_e
Transverse sound velocity	c_{TA}	4.2×10^3 m/s
Longitudinal sound velocity	c_{LA}	6.7×10^3 m/s
TA	Ξ_{TA}	1.5 eV
LA	Ξ_{LA}	2.4 eV
Piezoelectric constant	e_{11}	3.0×10^{-11} C/m

APPENDIX E: PARAMETERS USED IN THE CALCULATIONS

The parameters for MoS_2 are given in Table I.

[1] D. Xiao, G.-B. Liu, W. Feng, X. Xu, and W. Yao, Phys. Rev. Lett. **108**, 196802 (2012).

[2] X. Xu, W. Yao, D. Xiao, and T. F. Heinz, Nat. Phys. **10**, 343 (2014).

[3] X.-Q. Yu, Z.-G. Zhu, Gang Su, and A.-P. Jauho, Phys. Rev. Lett. **115**, 246601 (2015).

[4] K. F. Mak, K. L. McGill, J. Park, and P. L. McEuen, Science **344**, 1489 (2014).

[5] Q. H. Wang, K. Kalantar-Zadeh, A. Kis, J. N. Coleman, and M. S. Strano, Nat. Nanotechnol. **7**, 699 (2012).

[6] K. S. Novoselov, D. Jiang, F. Schedin, T. J. Booth, V. V. Khotkevich, S. V. Morozov, and A. K. Geim, Proc. Natl. Acad. Sci. U.S.A. **102**, 10451 (2005).

[7] B. Radisavljevic, A. Radenovic, J. Brivio, V. Giacometti, and A. Kis, Nat. Nanotechnol. **6**, 147 (2011).

[8] D. Wickramaratne, F. Zahid, and R. K. Lake, J. Chem. Phys. **140**, 124710 (2014).

[9] K. S. Bhargavi, S. Patil, and S. S. Kubakaddi, J. Appl. Phys. **118**, 044308 (2015).

[10] K. Kaasbjerg, K. S. Thygesen, and K. W. Jacobsen, Phys. Rev. B **85**, 115317 (2012).

[11] K. Kaasbjerg, K. S. Thygesen, and A.-P. Jauho, Phys. Rev. B **87**, 235312 (2013).

[12] D. K. Efetov and P. Kim, Phys. Rev. Lett. **105**, 256805 (2010).

[13] G. D. Mahan, *Many-Particle Physics* (Kluwer, New York, 2000).

[14] E. Cappelluti and L. Benfatto, Phys. Rev. B **79**, 035419 (2009).

[15] X.-Z. Yan, Y. Romiah, and C. S. Ting, Phys. Rev. B **77**, 125409 (2008).

[16] F. Bloch, Z. Phys. **59**, 208 (1930); E. Grüneisen, Ann. Phys. (Leipzig) **408**, 530 (1933); E. H. Hwang and S. Das Sarma, Phys. Rev. B **77**, 115449 (2008).

[17] H. Bruus and K. Flensberg, *Many-Body Quantum Theory in Condensed Matter Physics: An Introduction* (Oxford University Press, Oxford, 2004).
[18] J. S. Dugdale and Z. S. Basinski, Phys. Rev. **157**, 552 (1967).
[19] J. Bass, Adv. Phys. **21**, 431 (1972).
[20] T. Feng, B. Qiu, and X. Ruan, Phys. Rev. B. **92**, 235206 (2015).
[21] D. Stysiak, W. Borgie, and J. Deniszczyk, Phys. Status Solidi C **3**, 40 (2006).
[22] K. Kaasbjerg, J. H. J. Martiny, T. Low, and A.-P. Jauho, Phys. Rev. B **96**, 241411(R) (2017).