Analytical expressions of momentum matrix elements and spectrum broadening of extrinsic doped Dirac cone

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**1 author:**

Liubov Lokot

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1 Introduction

High-performance transistor operation of MoS$_2$ is suitable for realization on his base Ambipolar thin flake transistors. Let us known that the high-performance transistor known via high Hall effect measurements revealed mobility of 44 and 86 cm$^2$V$^{-1}$s$^{-1}$ for electrons and holes respectively [1]. In the paper [2] Integrated Circuits and Logic Operations are based on single-layer MoS$_2$. MoS$_2$ integrated circuits are capable of operations as inverters converting logical "1" into logical "0" making them suitable for incorporation into digital circuits.

In the papers [3, 4, 5] the electron-electron interaction effects in gated graphene sometimes also called extrinsic doped graphene were considered.

Graphene/Ferroelectrics interface based integrated circuits and Logic Operations are capable of operations as inverters converting logical "1" into logical "0" at creating memory elements [6].

The single-layer MoS$_2$ has a quantum luminescence efficiency and exhibits a high channel mobility like metallic one (200 cm$^2$V$^{-1}$s$^{-1}$) and current ON/OFF ratio (10$^3$) when it was used as the channel materials in a field effect transistors (FET) and single-layer semiconductors materials for multifunctional optoelectronic device application [7].

It should be noted that the photoresponsivity from single-layer MoS$_2$ phototransistor can be equal as high as 7.5 mA/W under illumination $P_{light}$ = 80 $\mu$W and medium gate voltage $V_g$ = 50 V is better than that obtained from the single-layer graphene based FET (1 mA/W) [7].

Latter experiments have shown that MoS$_2$ is group-VI dichalcogenide crossovers a direct band-gap semiconductor only if single-layer is considered [8]. The inversion symmetry is broken in single layer MoS$_2$ and strong spin-orbit coupling is presented [8].

With the selected topics of the optical spectroscopy of highly excited semiconductors one can conclude by illustratively that practically definition of physics of highly excited semiconductors is determined by many-body effects [9, 10, 11, 12, 13, 14, 15, 16, 17, 18, 19, 20, 21, 22, 23, 24, 25, 26, 27]. Green function techniques are best suited for that purpose [9].

In section 2 We considered the expressions of energy spectrums and wave functions with chiral band dispersion for materials with "Mexican hat"-type spectrums.

In section 3 We derived of expressions of momentum matrix elements for MoS$_2$.

In section 4 We found the analytical expressions for broadening of spectrum of extrinsic doped Dirac cone in on-shell approximation of self energy. On-shell approximation of self energy calculations are based on the Bethe-Salpeter equations.
2 Derivation of expressions of energy spectrums and wave functions with chiral band dispersion for materials with "Mexican hat" shape of band spectrum

The Schrödinger equations for calculating of energy spectrums and wave functions with chiral band dispersion for materials with "Mexican hat" shape of band dispersion can be written in the following general form:

\[
\begin{pmatrix}
\frac{\hbar^2}{2m_t} k^2_i - e & \alpha^*(k_y + i k_x) \\
\alpha^*(k_y - i k_x) & \frac{\hbar^2}{2m_t} k^2_i - e
\end{pmatrix}
\begin{pmatrix}
C_1 \\
C_2
\end{pmatrix} = 0.
\]  

(1)

The exact solutions of which for energy spectrums can be found in the following form

\[\epsilon = \frac{\hbar^2}{2m_t} k^2_i - \epsilon \pm (\alpha^*)^2 k^2_i = 0,\]

(2)

\[\epsilon_{\pm} = \frac{\hbar^2}{m_t} k^2_i \pm \sqrt{\left(\frac{\hbar^2}{m_t} k^2_i\right)^2 - 4\left(\frac{\hbar^2}{2m_t} k^2_i - (\alpha^*)^2 k^2_i\right)} = \frac{\hbar^2}{2m_t} k^2_i \pm \alpha^* k_1,\]

(3)

\[\epsilon_+ = \left(\frac{\hbar}{\sqrt{2m_t}} k_1 + \frac{1}{2} \frac{\sqrt{2m_t}}{\hbar} \alpha^*\right)^2 - \frac{2m}{\hbar^2} \frac{1}{4} (\alpha^*),\]

(4)

\[\epsilon_- = \left(\frac{\hbar}{\sqrt{2m_t}} k_1 - \frac{1}{2} \frac{\sqrt{2m_t}}{\hbar} \alpha^*\right)^2 - \frac{2m}{\hbar^2} \frac{1}{4} (\alpha^*).\]

(5)

The exact solutions of Schrödinger equations for wave functions with chiral band dispersion can find as follows

\[\frac{\hbar^2}{2m_t} k^2_i - \epsilon_{\pm})C_1 + \alpha^*(k_y + i k_x)C_2 = 0,\]

(6)

\[C_1 = \frac{\alpha^*(k_y + i k_x)}{\frac{\hbar^2}{2m_t} k^2_i - \epsilon_+} C_2,\]

(7)

Having regard to the condition of normalizable eigenfunctions

\[|C_1|^2 + |C_2|^2 = 1,\]

(8)

from the equation

\[\frac{(\alpha^*)^2 k^2_i}{\left(\frac{\hbar^2}{2m_t} k^2_i - \epsilon_+\right)^2} C_2^2 + C_2^2 = 1,\]

(9)

\[C_2 = \frac{1}{\sqrt{1 + \frac{(\alpha^*)^2 k^2_i}{\left(\frac{\hbar^2}{2m_t} k^2_i - \epsilon_+\right)^2}}} = \frac{1}{\delta},\]

(10)

the wave normalizable eigenfunctions with chiral band dispersion for the state \(\epsilon_+\) was found as follows

\[\left|\frac{\alpha^*(k_y + i k_x)}{\frac{\hbar^2}{2m_t} k^2_i - \epsilon_+}\right| = \frac{1}{\delta},\]

(11)

The other wave normalizable eigenfunctions with chiral band dispersion for the state \(\epsilon_-\) was found as follows

\[\alpha^*(k_y - i k_x)C_1 + \left(\frac{\hbar^2}{2m_t} k^2_i - \epsilon_-\right)C_2 = 0,\]

(12)

\[C_2 = -\frac{\alpha^*(k_y - i k_x)}{\frac{\hbar^2}{2m_t} k^2_i - \epsilon_-} C_1,\]

(13)

\[|C_1|^2 + |C_2|^2 = 1,\]

(14)

\[\frac{(\alpha^*)^2 k^2_i}{\left(\frac{\hbar^2}{2m_t} k^2_i - \epsilon_-\right)^2} C_2^2 + C_2^2 = 1,\]

(15)
Derivation of expressions of momentum matrix elements for MoS$_2$

The Schrödinger equations for calculating of energy spectrums and wave functions with chiral band dispersion for two-degenerate conduction band and spin-orbit splitting lower valence band can be written in the following form:

\[
\begin{vmatrix}
\frac{\hat{\Delta}}{2} - \epsilon \\
\epsilon
\end{vmatrix}
\begin{vmatrix}
\epsilon \\
\alpha t (k_x, t k_y)
\end{vmatrix}
= 0.
\]

The Schrödinger equations for calculating of energy spectrums and wave functions with chiral band dispersion for two-degenerate conduction band and spin-orbit splitting upper valence band can be written in the following form:

\[
\begin{vmatrix}
\frac{\hat{\Delta}}{2} - \epsilon \\
\epsilon
\end{vmatrix}
\begin{vmatrix}
\epsilon \\
\alpha t (k_x, t k_y)
\end{vmatrix}
= 0.
\]

The exact solutions of Schrödinger equations for energy spectrums for two-degenerate conduction band and spin-orbit splitting upper valence band can be written as follows

\[
-(\frac{\hat{\Delta}}{2} - \epsilon)(\frac{\hat{\Delta}}{2} + \epsilon) - a^2 t^2 (k_x^2 + k_y^2) = 0,
\]

\[
e_\pm = \pm \sqrt{\frac{\Delta^2}{4} + a^2 t^2 (k_x^2 + k_y^2)} = \pm \sqrt{\frac{\Delta^2}{4} + a^2 t^2 k_r^2}.
\]

Having regard to the condition of normalizable eigenfunctions the wave eigenfunctions with chiral band dispersion for the state $e_\pm$ were found as follows

\[
\left(\frac{\hat{\Delta}}{2} - e_+\right)C_1 + \alpha t (k_x, t k_y)C_2 = 0,
\]

\[
C_1 = -\frac{\alpha t (k_x, t k_y)}{\frac{\hat{\Delta}}{2} - e_+}C_2,
\]

\[
|C_1|^2 + |C_2|^2 = 1,
\]

\[
a^2 t^2 k_r^2 = \frac{(\frac{\hat{\Delta}}{2} - e_+)^2}{(\frac{\hat{\Delta}}{2} + e_-)^2}C_1^2 + C_2^2 = 1,
\]

\[
C_2 = \frac{1}{\sqrt{1 + \frac{a^2 t^2 k_r^2}{(\frac{\hat{\Delta}}{2} - e_+)^2}}} = \frac{1}{\delta},
\]

\[
\begin{vmatrix}
-\frac{\alpha t (k_x, t k_y)}{\frac{\hat{\Delta}}{2} + e_-} \\
\frac{\hat{\Delta}}{2} + e_-
\end{vmatrix}
\begin{vmatrix}
\frac{1}{\delta} \\
-\Gamma \exp^{\rho}
\end{vmatrix}
= 0,
\]

\[
at (k_x + t k_y)C_1 - (\frac{\hat{\Delta}}{2} + e_-)C_2 = 0.
\]
Let us know the following unitary matrices which consist of the found wave functions with chiral band dispersion

\[
C_2 = \frac{\text{at}(k_x + t k_y)}{\frac{\lambda}{2} - \epsilon_+} C_1, \quad \text{(31)}
\]

\[
|C_1|^2 + |C_2|^2 = 1, \quad \text{(32)}
\]

\[
+C_1^2 + \frac{a^2 t^2 k_i^2}{\left(\frac{\lambda}{2} - \epsilon_+\right)^2} C_1^2 = 1, \quad \text{(33)}
\]

\[
C_1 = \frac{1}{\sqrt{1 + \frac{a^2 t^2 k_i^2}{\left(\frac{\lambda}{2} - \epsilon_+\right)^2}}} = \frac{1}{\delta}, \quad \text{(34)}
\]

\[
\frac{1}{\delta} \left( \begin{array}{c}
\epsilon - \lambda \\
\frac{\lambda}{2} + \epsilon + \frac{1}{2} \sqrt{\frac{\lambda^2}{4} + \Delta^2 + 4a^2 t^2 k_i^2}
\end{array} \right), \quad \text{(35)}
\]

\[
\frac{1}{\delta} \left( \begin{array}{c}
-\frac{\lambda}{2} \\
\frac{\lambda}{2} + \epsilon - \frac{1}{2} \sqrt{\frac{\lambda^2}{4} + \Delta^2 + 4a^2 t^2 k_i^2}
\end{array} \right) \Gamma \exp^{-i\varphi}. \quad \text{(36)}
\]

The Schrödinger equations for energy spectrums for two-degenerate conduction band and spin-orbit splitting lower valence band can find as follows

\[
\frac{\Delta}{2} - \epsilon \left( \begin{array}{c}
\frac{\lambda}{2} + \epsilon \\
\frac{\lambda}{2} + \epsilon + a^2 t^2 k_i^2
\end{array} \right) C_1 = 0. \quad \text{(38)}
\]

The exact solutions of Schrödinger equations for energy spectrums for two-degenerate conduction band and spin-orbit splitting lower valence band can find as follows

\[
-(\frac{\Delta}{2} - \epsilon)(\frac{\Delta}{2} + \frac{\lambda}{2} + \epsilon) - a^2 t^2 k_i^2 = 0, \quad \text{(39)}
\]

\[
\epsilon_{\pm} = -\frac{\lambda}{4} \pm \frac{1}{2} \sqrt{\frac{\lambda^2}{4} + \Delta^2 + 4a^2 t^2 k_i^2}, \quad \text{(40)}
\]

Having regard to the condition of normalizable eigenfunctions the wave eigenfunctions with chiral band dispersion for the state \(\epsilon_{\pm}\) were found as follows

\[
\frac{\Delta}{2} - \epsilon_+ C_1 + \text{at}(k_x - t k_y) C_2 = 0, \quad \text{(41)}
\]

\[
\frac{\frac{\lambda}{2} + \epsilon - \frac{1}{2} \sqrt{\frac{\lambda^2}{4} + \Delta^2 + 4a^2 t^2 k_i^2}}{\delta} C_1 = \text{at}(k_x + t k_y) C_2, \quad \text{(42)}
\]

\[
\frac{\Delta}{2} - \epsilon_- C_1 + \text{at}(k_x + t k_y) C_2 = 0, \quad \text{(43)}
\]

\[
\frac{\frac{\lambda}{2} - \epsilon_+ + \frac{1}{2} \sqrt{\frac{\lambda^2}{4} + \Delta^2 + 4a^2 t^2 k_i^2}}{\delta} C_1 = \text{at}(k_x - t k_y) C_2. \quad \text{(44)}
\]

Let us know the following unitary matrices which consist of the found wave functions with chiral band dispersion

\[
\hat{U} = \frac{1}{\delta} \left( \begin{array}{c}
1 \\
-\Gamma \exp^{i\varphi}
\end{array} \right), \quad \text{(45)}
\]

\[
\hat{U}^{-1} = \delta \left( \begin{array}{c}
\frac{1}{\Gamma \exp^{i\varphi}} \\
\frac{1}{\Gamma \exp^{i\varphi}}
\end{array} \right) \frac{1}{\Gamma \exp^{i\varphi}}. \quad \text{(46)}
\]
\[ \hat{U}^{-1} = \begin{vmatrix} 1 & 0 \\ 0 & 1 \end{vmatrix}, \] 
\[ \Gamma = \frac{\Delta k}{\frac{\Delta}{2} - \sqrt{\frac{\Delta^2}{4} + a^2 t^2 k_i^2}}, \] 
for the considered MoS\textsubscript{2} Hamiltonian can realize unitary transformations using found unitary matrixes
\[ \hat{H} = \begin{vmatrix} \frac{\Delta}{2} & atk_i \exp^{-i\varphi} \\ atk_i \exp^{i\varphi} & -\frac{\Delta}{2} \end{vmatrix}, \] 
Hence the diagonal Hamiltonian one can consider as follows
\[ \hat{V} = \hat{U} \hat{H} \hat{U}^{-1}, \] 
\[ \hat{V} = \begin{vmatrix} \sqrt{\frac{\Delta^2}{4} + a^2 t^2 k_i^2} & 0 \\ 0 & \sqrt{\frac{\Delta^2}{4} + a^2 t^2 k_i^2} \end{vmatrix}, \] 
In the paper [28] the expressions for momentum matrix elements were presented in the following general form:
\[ \langle \Psi_\pm | e \hat{U} \frac{\partial \hat{H}}{\partial \mathbf{k}} \hat{U}^{-1} | \Psi_\mp \rangle, \] 
where e gives polarization of incident light.
One can derivate the expressions for calculation of momentum matrix elements for interband transitions as well as intraband transitions in stimulated emission explaining
\[ \frac{\partial \hat{U} \hat{U}^{-1}}{\partial \varphi} = \hat{U} \hat{H} \hat{U}^{-1} + \frac{\partial \hat{U} \hat{U}^{-1}}{\partial \varphi} \]
\[ = \hat{U} \hat{H} \hat{U}^{-1} \frac{\partial \hat{U} \hat{U}^{-1}}{\partial \varphi} + \frac{\partial \hat{U} \hat{U}^{-1}}{\partial \varphi} \]
\[ = \hat{U} \hat{H} \frac{\partial \hat{U} \hat{U}^{-1}}{\partial \varphi} + \frac{\partial \hat{U} \hat{U}^{-1}}{\partial \varphi} \]
Since
\[ \hat{U} \hat{U}^{-1} = \mathbb{I}, \] 
as well as using
\[ \frac{\partial \hat{U} \hat{U}^{-1}}{\partial \varphi} = 0, \] 
\[ \hat{U} \frac{\partial \hat{U} \hat{U}^{-1}}{\partial \varphi} + \frac{\partial \hat{U} \hat{U}^{-1}}{\partial \varphi} = 0, \] 
one can find the following unitary transformation for momentum
\[ \hat{U} \frac{\partial \hat{H}}{\partial \mathbf{k}} \hat{U}^{-1} = \frac{\partial \hat{U} \hat{H} \hat{U}^{-1}}{\partial \mathbf{k}} + \hat{H} \hat{U}^{-1} \frac{\partial \hat{U}}{\partial \mathbf{k}} - \hat{U}^{-1} \frac{\partial \hat{U}}{\partial \mathbf{k}} \hat{H}, \] 
Since
\[ \frac{\partial \hat{H}}{\partial \mathbf{k}} = \frac{1}{k_i} \frac{\partial \hat{k}_i \hat{H}_i}{\partial \mathbf{k}} + \frac{1}{k_i} \frac{\partial \hat{H}_\varphi}{\partial \varphi}, \] 
\[ \frac{\partial \hat{U}}{\partial \mathbf{k}} = \frac{1}{k_i} \frac{\partial \hat{k}_i \hat{U}_i}{\partial \mathbf{k}} + \frac{1}{k_i} \frac{\partial \hat{U}_\varphi}{\partial \varphi}, \] 
Therefore
\[ \hat{H}_i = \begin{vmatrix} -\sqrt{\frac{\Delta^2}{4} + a^2 t^2 k_i^2} & 0 \\ 0 & \sqrt{\frac{\Delta^2}{4} + a^2 t^2 k_i^2} \end{vmatrix} = \begin{vmatrix} -e_+ & 0 \\ 0 & e_+ \end{vmatrix}, \]
as well as

\[ \dot{U} = \frac{1}{\delta} \begin{bmatrix} 1 & -\Gamma \exp^{-\phi} \\ -\Gamma \exp^{-\phi} & 1 \end{bmatrix}, \]

where

\[ \Gamma = \frac{\Delta k_t}{\frac{\Delta}{2} - \sqrt{\frac{\Delta^2}{4} + a^2 t^2 k_t^2}}. \]

After the elementary algebra matrix transformations one can find

\[ \frac{\partial H}{\partial k} = \frac{H_{k_t}}{k_t} + \frac{\partial H}{\partial k_t} = \begin{bmatrix} \frac{-1}{k_t} \sqrt{\frac{\Delta^2}{4} + a^2 t^2 k_t^2} & 0 \\ 0 & \frac{1}{k_t} \sqrt{\frac{\Delta^2}{4} + a^2 t^2 k_t^2} \end{bmatrix} + \begin{bmatrix} -\frac{\Delta^2 k_t}{\frac{\Delta}{2} - \sqrt{\frac{\Delta^2}{4} + a^2 t^2 k_t^2}} & 0 \\ 0 & \frac{\Delta^2 k_t}{\frac{\Delta}{2} - \sqrt{\frac{\Delta^2}{4} + a^2 t^2 k_t^2}} \end{bmatrix}, \]

\[ \frac{\partial H}{\partial k} = \begin{bmatrix} \frac{-\Delta k_t}{k_t} \exp^{-\phi} - \frac{\Delta^2 k_t}{\frac{\Delta}{2} - \sqrt{\frac{\Delta^2}{4} + a^2 t^2 k_t^2}} \exp^{-\phi} \\ 0 \end{bmatrix}, \]

\[ \frac{\partial U}{\partial k_t} = \frac{U}{k_t} + \frac{\partial U}{\partial k_t} + \frac{1}{k_t} \frac{\partial U}{\partial \phi}, \]

\[ \frac{\partial U}{\partial k_t} = \frac{\partial U}{\partial k_t} = \begin{bmatrix} \frac{-\Gamma \exp^{-\phi}}{k_t} - \frac{\Delta k_t}{k_t} \exp^{-\phi} + \frac{\Delta^2 k_t}{\frac{\Delta}{2} - \sqrt{\frac{\Delta^2}{4} + a^2 t^2 k_t^2}} \exp^{-\phi} \end{bmatrix}. \]

Also keeping in mind and realizing the following algebra matrix transformation one can find

\[ \hat{H} U^{-1} = \begin{bmatrix} \frac{\Delta}{2} & at(k_x - \xi k_y) \\ -\frac{\Delta}{2} & \frac{1}{k_t} \sqrt{\frac{\Delta^2}{4} + a^2 t^2 k_t^2} - \frac{\Gamma \exp^{-\phi}}{1 + t^2} \exp^{-\phi} \end{bmatrix}, \]

\[ \frac{\partial U}{\partial k} = \begin{bmatrix} \frac{-\Gamma \exp^{-\phi}}{k_t} - \frac{\Delta k_t}{k_t} \exp^{-\phi} + \frac{\Delta^2 k_t}{\frac{\Delta}{2} - \sqrt{\frac{\Delta^2}{4} + a^2 t^2 k_t^2}} \exp^{-\phi} \\ \frac{1}{k_t} \sqrt{\frac{\Delta^2}{4} + a^2 t^2 k_t^2} \exp^{-\phi} \end{bmatrix}, \]

\[ \frac{\partial U}{\partial k_t} = \begin{bmatrix} \frac{-\Gamma \exp^{-\phi}}{k_t} - \frac{\Delta k_t}{k_t} \exp^{-\phi} + \frac{\Delta^2 k_t}{\frac{\Delta}{2} - \sqrt{\frac{\Delta^2}{4} + a^2 t^2 k_t^2}} \exp^{-\phi} \\ \frac{1}{k_t} \sqrt{\frac{\Delta^2}{4} + a^2 t^2 k_t^2} \exp^{-\phi} \end{bmatrix}. \]
Emission spectrum broadening of asymptotic Dirac cone of MoS$_2$  

In the paper the found emission spectrum broadening are shown to be formulated as reciprocal magnitude of quasiparticle lifetime which are directly calculated via imaginary part of self energy of asymptotic Dirac cone of MoS$_2$. In the paper [9] the imaginary part of self energy in asymptotic Dirac cone due to electron-electron interaction was determined as

$$3\Sigma_q(k,\omega) = -\frac{1}{2}\sum_{q',s'=\pm} V_q [n_B(\xi_{k+q'+s'-}\omega) + n_F(\xi_{k+q,s})] \times (1 + ss' \cos \theta) 3\epsilon(q,\xi_{k+q,s} - \omega),$$

where quasiparticle lifetime can be directly calculated via imaginary part of self energy of asymptotic Dirac cone of MoS$_2$

$$\frac{1}{\tau} = \Gamma_s(k) = 23\Sigma_q(k,\xi_{k,s}),$$

where MoS$_2$ is asymptotically presented via Dirac cone, where $\epsilon_k = \hbar v_F |k|$, $\mu$ is chemical potential, $n_B$, $n_F$ are Bose-Einshtein and Fermi-Dirac distribution functions correspondingly.

$$\epsilon(q,\omega) = 1 + V_q \Pi(q,\omega),$$

is dynamical dielectric function calculated via Lindhard formula, where

$$V_q = \frac{2\pi e^2}{\kappa q},$$

One can find the following expression for matrix in the form with taking into consideration equation (63) can be found seeking the momentum matrix elements

$$\tilde{B} = \tilde{H}^{-1} \frac{\partial \tilde{U}}{\partial k} - U^{-1} \frac{\partial \tilde{U}}{\partial k} \tilde{H},$$

$$B_{11} = -at(1 - \Gamma + 2ak),$$

$$B_{12} = \Delta(A - \frac{\Gamma}{k^2}) \exp^{-i\varphi} - \frac{\Delta \Gamma}{k^2} \exp^{-i\varphi} + atk, \exp^{-i\varphi}(-A - \frac{\Gamma}{k^2}) + atk, \exp^{-i\varphi}(A - \frac{\Gamma}{k^2}),$$

$$B_{21} = -\frac{\Delta \Gamma}{k^2} \exp^{-i\varphi} + at^2, \exp^{-i\varphi} - \Delta(-A - \frac{\Gamma}{k^2}) \exp^{-i\varphi},$$

$$B_{22} = -2at^2, \exp^{-i\varphi} - 2at, \exp^{-i\varphi},$$

$$\frac{\Delta \Gamma}{k^2} \exp^{-i\varphi} + atk, \exp^{-i\varphi} - \Delta(A - \frac{\Gamma}{k^2}) \exp^{-i\varphi}.$$
Coulomb interaction in momentum space, \( \kappa \) is dielectric constant of host medium, \( \Pi(q, \omega) \) is polarization function. Imaginary part of self energy for extrinsic doped materials with dispersion of asymptotic Dirac cone \( \epsilon_F \gg \xi_k \). In approximation \( \omega = \xi_k \) as well as zero temperature \( T = 0 \) \( \omega \) can be calculated via Heaviside dimensionless unit step function as follows

\[
\omega = \xi_k, \quad T = 0,
\]

(86)

\[
3\Sigma_i(k, \xi_k) = \frac{1}{2} \sum_{q, q' = \pm} V_q [\Theta(\epsilon_k - s' \epsilon_{k+q}) - \Theta(-\xi_k + \epsilon_{q'})] \times (1 + s' \cos \theta) 3 \epsilon(q, q, q_{\xi_k} - \epsilon_{q'; 0}^0).
\]

(87)

Let us known the polarizational propagator function

\[
\Pi(q, \omega) = -\frac{g_s g_v}{L^2} \sum_{k, s, \xi} \frac{f_{s, k} - f_{s', k'}}{\omega + \epsilon_k - \epsilon_{s', k'} + i \eta} \epsilon_{s'}(k'),
\]

(88)

where

\[
\frac{f_{s, k} (1 - \cos \Theta_{kk})}{\omega + \epsilon_k + \epsilon_{k'} + i \eta} = \frac{f_{s, k} (1 - \cos \Theta_{kk})}{\omega + \epsilon_k - \epsilon_{k'} - i \eta} \pi \delta(\omega + \epsilon_k - \epsilon_{k'}).
\]

(89)

Let us known

\[
\frac{f_{s, k} (1 - \cos \Theta_{kk})}{\omega + \epsilon_k + \epsilon_{(k+q) +} + i \eta},
\]

(90)

in which

\[
f_{s, k} (1 - \cos \Theta_{kk'}) \delta(\omega + \epsilon_k + \epsilon_{(k+q)+}) = \frac{(1 - \cos \Theta_{kk'})}{1 + \exp[^{\frac{\omega - \epsilon_{(k+q) +}}{2 \epsilon_F}]} \delta(\omega + 2 \epsilon_F k + \frac{q}{2}),
\]

(91)

the expression for energy can expand in Taylor series as follows

\[
\epsilon_{(k+q)_+} = \epsilon_k + \frac{\partial \epsilon_k}{\partial k} q.
\]

(92)

Let us known the polarizational propagator integral:

\[
\frac{1}{E_F (1 - \cos \Theta_{kk})} \delta(\frac{\omega}{E_F} + 2 \frac{k}{k_y} + \frac{q}{k_y}),
\]

(93)

as well as

\[
\frac{1}{E_F (1 - \cos \Theta_{kk})} \delta(\frac{\omega}{E_F} + 2 \frac{k}{k_y} + \frac{q}{k_y}),
\]

(94)

in two-dimensional space

\[
\int k dk d\Theta \frac{1}{E_F (1 - \cos \Theta)} \delta(\frac{\omega}{E_F} + 2 \frac{k}{k_y} + \frac{q}{k_y}),
\]

(95)

one can find after elementary mathematical transformations

\[
\frac{1}{E_F (1 - \cos \Theta_{kk})} \delta(\frac{\omega}{E_F} + 2 \frac{k}{k_y} + \frac{q}{k_y}) \frac{k^2}{2 E_F} = -2 \pi \frac{k^2}{2 E_F} \Theta(2 + \frac{\omega}{E_F} + \frac{q}{k_y}) \Theta(\frac{\omega}{4 E_F} + \frac{q}{4 k_y} + \frac{q}{2}).
\]

(96)

Let us known the following integral also

\[
\frac{1}{E_F (1 - \cos \Theta_{kk})} \delta(\frac{\omega + \epsilon_{(k+q)+}}{E_F (1 - \cos \Theta_{kk})}) = \frac{1}{1 + \exp^{\frac{\omega - \epsilon_{(k+q)+}}{2 \epsilon_F}}} \delta(\omega + 2 \epsilon_F k + \frac{q}{2}).
\]

(97)

as well as
\[ \Pi_2 = \int (1 - \cos \theta) d\theta \int d\mathbf{k} k^2 \frac{1/r}{(r^2 + r^2 + r^2)} \Theta\left(\frac{\omega}{2k_F} + \frac{k}{2k_F} + \frac{q}{2k_F} + \frac{\nu}{2}\right) = k_F^2 \pi \int \frac{k}{k_F} \frac{d}{d\mathbf{k}} \frac{1/r}{(r^2 + r^2 + r^2)} \Theta\left(\frac{\omega}{2k_F} + \frac{k}{2k_F} + \frac{q}{2k_F} + \frac{\nu}{2}\right). \]  

(98)

Since
\[ \int \frac{k}{k_F} \frac{d}{d\mathbf{k}} \frac{1/r}{(r^2 + r^2 + r^2)} = (\frac{\omega}{2k_F} + \frac{k}{2k_F} + \frac{q}{2k_F}) - (\frac{\omega}{2k_F} + \frac{q}{2k_F}) \ln(\frac{\omega}{2k_F} + \frac{k}{2k_F} + \frac{q}{2k_F}), \]

(99)

where
\[ \frac{k}{k_F} = -\frac{\omega}{E_F} - \frac{q}{k_F} - \nu_F. \]

(100)

So the polarizational propagator \( \Pi_2 \) is found in the form:
\[ \Pi_2 = k_F^2 \pi (-\frac{\omega}{2k_F} - \frac{q}{k_F} - \nu_F) - (\frac{\omega}{2k_F} + \frac{q}{2k_F}) \ln(-\frac{\omega}{2k_F} - \frac{q}{2k_F} - \nu_F)) \times \Theta\left(\frac{\omega}{2k_F} + \frac{q}{2k_F} + \frac{\nu}{2} + \frac{1}{2}\right). \]

(101)

The absolute value of wave vector one can expand in Taylor series as follows
\[ |\mathbf{k} + \mathbf{q}| = |\mathbf{k}| + \frac{\partial |\mathbf{k}|}{\partial \mathbf{q}}. \]

(102)

Let us known the screening Coulomb potential
\[ W_q = \frac{V_q}{1 + V_q \Pi_2 - i \pi V_q \Pi_1} = V_q (1 - V_q \Pi_2 + i \pi V_q \Pi_1), \]

(103)

where
\[ \Pi_1 = -2\pi \frac{k_F^2}{2E_F} (\frac{\omega}{2k_F} + \frac{q}{2k_F}) \Theta(2 + \frac{\omega}{E_F} + \frac{q}{4k_F} + \frac{\nu}{2}), \]

(104)

\[ \Pi_2 = k_F^2 \pi ((-\frac{\omega}{2k_F} - \frac{q}{k_F} - \nu_F) - (\frac{\omega}{2k_F} + \frac{q}{2k_F}) \ln(-\frac{\omega}{2k_F} - \frac{q}{2k_F} - \nu_F)) \Theta(\frac{\omega}{2k_F} + \frac{q}{2k_F} + \frac{\nu}{2} + \frac{1}{2}). \]

(105)

In general form of self energy
\[ \Sigma(k, \omega) = -\frac{1}{\beta} \sum_n \sum_{\nu} G_{\nu n} (k + q, \omega + \imath \nu_n) W_q (q, \nu_n) F_{\nu n} (k + q), \]

(106)

where
\[ V_q (1 - V_q \Pi_2 + i \pi V_q \Pi_1) \frac{F_{\nu n} (k + q)}{\epsilon(k) + \imath \nu_n - \epsilon(k + q) + \mu}, \]

(107)

as well as Green function one can rewrite like
\[ \frac{1}{\epsilon(k) + \imath \nu_n - \epsilon(k + q) + \mu} = \frac{1}{\epsilon(k) - \epsilon(k + q) + \mu} - \imath \pi \delta(\epsilon(k) - \epsilon(k + q) + \mu) \]

(108)

Let us known the self energy integral:
\[ \frac{S}{(2\pi)^2} = \frac{S}{(2\pi)^2} \int q d q d \theta V_q (1 - V_q \Pi_2) F_{\nu n} (k + q) \delta(\epsilon(k) - \epsilon(k + q) + \mu) - \int q d q d \theta \frac{V_q \Pi_1 (k, k + q)}{\epsilon(k) - (\epsilon(k) + \mu)}. \]

(109)

The selected part of integral with the propagator \( \Pi_1 \) has the form:
\[ \int q d q d \theta \frac{V_q \Pi_1 (k, k + q)}{\epsilon(k) - (\epsilon(k) + \mu)} = \int q d q d \theta (2\pi)^2 \frac{\exp^2}{(\epsilon(k) - (\epsilon(k) + \mu)} \Theta(2 + \frac{\omega}{E_F} + \frac{q}{4k_F} + \frac{\nu}{2}) \Theta(\frac{\omega}{2k_F} + \frac{q}{2k_F} + \frac{\nu}{2}) \left(-\frac{1}{\epsilon(k) - (\epsilon(k) + \mu)}\right) \]

(110)
the solution of which we seek like

Let us known the self energy integral:

\[
\int q dq d\theta V_q (1 - V_q \Pi_2) F_{\nu'}(k, k + q) \delta(e(k) - e(k + q) + \mu) .
\]  

(112)

The selected part of integral with the propagator \( \Pi_2 \) has the form:

\[
\int q dq d\theta V^2_{q} \Pi_2 F_{\nu'}(k, k + q) \delta(e(k) - e(k + q) + \mu) =
\]

\[
= \int q dq d\theta \frac{(2\pi^2)^2}{k_F^2} \pi ((-\frac{v_F}{2k_F} - \frac{\Delta}{2k_F} - \nu_F) - \frac{q}{2k_F} \ln(-\frac{v_F}{2k_F} - \frac{q}{2k_F} - \nu_F)) \Theta(\frac{q}{2k_F} + \frac{v_F}{2} + \frac{\Delta}{2} + \frac{1}{2})
\times F_{\nu'}(k, k + q) \delta(e(k) - e(k + q) + \mu),
\]

(113)

the solution of which we seek like

\[
\int \frac{1}{2} d \frac{d^4 q}{k_F} \frac{d^4 \theta}{k_F} (2\pi^2)^2 \pi ((-\frac{v_F}{2k_F} - \frac{\Delta}{2k_F} - \nu_F) - \frac{q}{2k_F} \ln(-\frac{v_F}{2k_F} - \frac{q}{2k_F} - \nu_F)) \Theta(\frac{q}{2k_F} + \frac{v_F}{2} + \frac{\Delta}{2} + \frac{1}{2})
\times \frac{\Delta}{2} \frac{\frac{v_F}{2} - \frac{\Delta}{2} + \frac{1}{2}}{\Delta \frac{2(1 + 2t^2) - \frac{\Delta}{2}}} =
\]

\[
= 2\pi \int \frac{1}{2} d \frac{d^4 q}{k_F} \frac{d^4 \theta}{k_F} (2\pi^2)^2 \pi ((-\frac{v_F}{2k_F} - \frac{\Delta}{2k_F} - \nu_F) - \frac{q}{2k_F} \ln(-\frac{v_F}{2k_F} - \frac{q}{2k_F} - \nu_F)) \Theta(\frac{q}{2k_F} + \frac{v_F}{2} + \frac{\Delta}{2} + \frac{1}{2})
\times \delta(-\frac{\Delta}{2} + \frac{\Delta}{2} + \frac{1}{2}).
\]

(114)

So the imaginary part of self energy (87) with propagator \( \Pi_2 \) of extrinsic doped Dirac cone in on-shell approximation is reduced into the quadrature formula.

## 5 Appendix

\[
V = \frac{\Delta}{2} \frac{\frac{v_F}{2} - \frac{\Delta}{2}}{\Delta \frac{2(1 + 2t^2) - \frac{\Delta}{2}}} \]

(115)

\[
\hat{V} = \hat{U} \hat{V} \hat{U}^{-1},
\]

(116)

\[
V = \frac{1}{\Gamma} \exp^{-i\phi} \Gamma \exp^{-i\phi}
\]

(117)

\[
V_{11} = \frac{1}{4} \frac{\frac{\Delta}{2} + \Delta^2 + \frac{\Delta}{2} - \frac{\Delta}{2}}{4} + a^2 \frac{t^2}{2},
\]

(118)

\[
V_{12} = 0,
\]

(119)

\[
V = \frac{1}{4} \frac{\Delta^2 + a^2 t^2 k_t^2}{4} + \frac{\Delta^2 + a^2 t^2 k_t^2}{4}
\]

(120)

Table 1. The lattice constant \( a \) in \( \text{Å} \), the effective hopping integral \( t \) in eV, the energy of gap \( \Delta \) in eV, the spin splitting at the valence band top caused by the spin-orbit coupling \( 2\lambda \) in eV.

<table>
<thead>
<tr>
<th>Material</th>
<th>( a )</th>
<th>( t )</th>
<th>( \Delta )</th>
<th>( 2\lambda )</th>
</tr>
</thead>
<tbody>
<tr>
<td>MoS(_2)</td>
<td>3.193</td>
<td>1.66</td>
<td>1.10</td>
<td>0.15</td>
</tr>
</tbody>
</table>
6 Summary

In the paper [3] the inelastic quasiparticle lifetime of extrinsic doped graphene was calculated and the analytical expressions for the on-shell imaginary part of the self energy for the Dirac cone were found. The broadening spectrum of extrinsic doped Dirac cone was related with the Uncertainty Heisenberg principle $\Delta E \Delta t \geq \frac{\hbar}{2}$. It means that thin spectrum is connected with rapid optical inter- and intraband transitions. Because the Coulomb electron-electron interaction leads to the inelastic quasiparticle lifetime of extrinsic doped Dirac cone and as consequence can describe weak localization effects in quantum condensed matter at zero temperature with allowed laser excited optical transitions. On-shell approximation of self energy calculations are based on the Bethe-Salpeter equations in Green function techniques [29, 30].

We found the analytical expressions for broadening of spectrum of extrinsic doped Dirac cone in on-shell approximation of self energy.

The imaginary part of self energy is equal commensurately of several Fermi energy $E_F$ for carrier density from $10^{10}$ cm$^{-2}$, $10^{11}$ cm$^{-2}$ to $10^{12}$ cm$^{-2}$ for temperatures from 0K, 50K, 100K [3]. Hence MoS$_2$ is suitable for realization on his base Ambipolar MoS$_2$ thin flake transitions [1]. The hole mobility is twice the value of the electron mobility and accumulated carrier density arrived $10^{14}$ cm$^{-2}$ which is on one order value larger then conventional semiconductor Field Effect Transistors. So hight mobility of carrier as well as hight carrier density are suitable for classification MoS$_2$ channel transport like metallic.

References