Modeling the electron-photon interaction in monolayers of graphene and transition metal dichalcogenides in a tight binding approximation

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Abstract. In the presence of a strong electromagnetic field, the spectrum of charge carriers in a Dirac material is changed. The interaction of a linearly polarized field with electrons in the Dirac material leads to anisotropy. The anisotropy axis coincides with the direction of the electric field in the linearly polarized wave. We show that the major contribution to the interaction of electrons with an electromagnetic field comes from elastic scattering processes, whereas taking into account inelastic processes leads to an error of about 2%.

1. Introduction
Monolayers of transition metal dichalcogenides (TMDC) are two-dimensional (2D) semiconductors, which have found applications in electronics and optics. The diverse applications in electronics are associated with the properties of a direct band gap, as distinct from indirect band gaps in three-dimensional layers of TMDC crystals. The monolayered TMDC have already begun to be used in field transistor, logic devices, and optoelectronic tunnel microscopes. The accumulation of experimental data and the drive towards the introduction of monolayer TMDC in real devices call for the development of theoretical models to describe their electronic properties. Such models are assumed to be detailed and concise at the same time, as well as containing a limited number of parameters while providing an accurate description.

The aim of this work is to develop a model to describe the photon-electron interaction in monolayers of TMDC. To be able to develop a mathematical model of the interaction of an electromagnetic field with TMDC monolayers one needs to rely on a model that describes the charge carrier behavior in the absence of an electromagnetic field. A review of the models discussed in Refs. [1 - 11] is given in the first section of this work. Based on the approach developed in those papers it is possible to construct a model Hamiltonian that would describe the behavior of charge carriers in TMDC in the absence of an electromagnetic field. We use it to construct a Hamiltonian of the interaction of an external field with charge carriers inside the TMDC [12]. Next, the interaction of a periodic electromagnetic field with electrons is analyzed.
The behavior of a quantum system can essentially change under the action of a periodic perturbation. The key parameter that determines the character of the system interaction with an external field is the ratio of the perturbation frequency to a characteristic energy scale of the system. In the case of slow modulation, i.e., when the perturbation field frequency is much lower than the characteristic energy scale of the system, an adiabatic theorem proposed by V. Fock can be employed. The theorem states that a physical system remains in an instantaneous eigenstate if a given time-varying perturbation is acting on it slowly enough. Then, time can be interpreted as a parameter that defines parameters of the Hamiltonian. That is, if there is a stationary Hamiltonian $H_0(\lambda)$, where $\lambda$ is a set of parameters, whose eigenenergies and eigenstates are known:

$$H_0(\lambda) \psi_n(\lambda) = \varepsilon_n(\lambda) \psi_n(\lambda),$$

then, the non-stationary equation for the Hamiltonian

$$H(t) = H_0(\lambda) + V(t)$$

can be represented as a stationary $\tilde{H}(\tilde{\lambda}(t))$, whereas the eigenfunctions and eigenenergies are derived from the solution of a stationary equation

$$\tilde{H}(\tilde{\lambda}(t))\psi_n(\tilde{\lambda}(t)) = \varepsilon_n(\tilde{\lambda}(t))\psi_n(\tilde{\lambda}(t)).$$

If, however, the field frequency is close to that defining a certain inter-level transition energy in the system, the pattern changes drastically; for instance, if a two-level system interacts with an electromagnetic field whose frequency is close to that of the inter-level transition in the system, there occur inter-level Rabi oscillations, whose frequency depends on the dipole moment of the two-level system. Finally, for a high-frequency field, by averaging the dynamic properties of the system over period, we also obtain a quasi-periodic problem

$$i\frac{\partial \psi(t)}{\partial t} = H(t)\psi(t) \rightarrow i\tilde{\varepsilon} \tilde{\psi} = \tilde{H}\tilde{\psi}.$$ 

Properties of an effective quasi-stationary Hamiltonian can be essentially different from those of a free-system Hamiltonian. Thus, it is possible to construct new Hamiltonians and, consequently, new states of matter by applying a periodic excitation. The external high-frequency field creates artificial calibration fields, which change base characteristics of effective static Hamiltonians for the system. This approach is known as Focke engineering or electromagnetic dressing. In the case of a dressing electromagnetic field, this approach has been actively employed in both atomic physics and physics of condensed matter. It has proven to offer an instrument for flexibly controlling not only local spectral properties of a system -- such as an effective mass of quasiparticle, group velocity, and conduction but also its global topological properties [12].

2. Electronic structure of monolayers of transition metal dichalcogenides

Below, we give a brief outline of the electronic structure of monolayer transition metal dichalcogenides. It is worth noting that properties of monolayers of TMDC are similar to those of monolayers of graphene.

Like graphene, the group-IVB monolayer TMDCs of chemical composition MX$_2$ (where M=Mo or W and X=S, Se, Te) have hexagonal lattice structures and extrema (valleys). Of special interest is the behavior of dispersion relations in the valence and conduction bands (VB and CB) in the vicinity of the K and $\bar{K}$ points of the hexagonal Brillouin zone (BZ). Unlike graphene, the two-dimensional crystals have no inversion symmetry. In a standard approach to their theoretical modeling, monolayer TMDCs are mimicked as graphene with a staggered sub-lattice potential that breaks inversion symmetry. This approach describes some optical and transport effects related to the longitudinal degree of freedom of the electrons. Such an approach to describing graphene analogues [1] has been extended to obtain the tight-binding (TB) description of TMDCs. However, this approach has a number of essential shortcomings. An accurate description calls for the use of a large number of atomic orbitals. To account for the variations in weight of individual atomic orbitals in the band wave functions across the entire BZ, it is not only nearest-neighbor electron jumps that need to be taken into account.
The accumulation of experimental data and a drive towards introduction of monolayered TMCDs into practical electronic devices call for the development of theoretical models of their electronic properties. The sought-for models need to be detailed and compact simultaneously, containing a limited number of parameters and, at the same time, offering an accurate description.

In this work, the crystal structure of each MX$_2$ monolayer consists of three atomic layers, X – M – X. Within each layer, the M and X atoms form a hexagonal lattice: see figure 1. The M atoms in the middle plane have three nearest-neighbor X atoms both in the top and in the bottom layers, so that the crystal has D$_{3h}$ symmetry. The crystal structure is characterized by the in-plane lattice constant $a_0$ and the distance $d_{X,X}$ between the two chalcogene planes. It has been previously noted [2] that some details of the band structure obtained from density functional theory (DFT) calculations are rather sensitive to $a_0$ and $d_{X,X}$.

At present, the agreement with the existing experimental data has been achieved, e.g., regarding the relative effective mass at a BZ point or the energy difference $E_K$ between the tops of the VB at the K- and -K points. The agreement is only achieved if the values of $a_0$ and $d_{X,X}$ fall within a rather narrow interval.

![Figure 1. Structure of transition metal dichalcogenides. The plots are borrowed from Ref. [3].](image)

3. **An effective model in the vicinity of the K and -K points**

The behavior of the charge carriers has been most extensively studied, both experimentally and theoretically, in the vicinity of the K and -K points. The interest of researchers stems from the remarkable optical properties of these materials, which may be linked with the behavior of charge carriers at the K and -K points. The effect of spin-orbital coupling (SOC) at these points of the BZ turns out to be strong, leading to spin-splitting and spin-polarized bands. Considering that the K and -K points are linked by time reversal symmetry, polarization of the bands should be opposite for the K and -K points, which implies that spin and valley degrees of freedom are related in the manner described in Ref. [1].

In Ref. [3], base characteristics of the band structure were considered in terms of effective masses and spin splitting. Below, a detailed k • p theory is discussed, which reflects essential features of the DFT band structure and gives an insight into the results of recent experiments.

4. **Base characteristics of materials and their parameters**

An excellent review of the problem was proposed in Ref. [3]. It should be noted that there is a distinction between MoX$_2$ and WX$_2$ materials regarding the sign of the SOC constant in the CB (a microscopic explanation can be found in Refs. [4-6]). This distinction is important when interpreting the experiments in which properties of the A and B excitons are compared (for a detailed introduction in the exciton physics see Ref. [7]). Results of calculation of the effective masses and spin splitting obtained from DFT calculations were also discussed. In the works, the results of calculations and experiments were compared whenever possible.

One of the phenomena that initially attracted keen interest of researchers to the monolayer TMDCs was an explicit effect that the SOC had on the VB structure in the vicinity of the K and -K points. SOC leads to spin-splitting and spin-polarization of the VB, with the SOC-related energy scale amounting to several hundred meV: see Table 4 in Ref. [3]. For the first time, the SOC in the VB was studied using DFT calculations. The results obtained can be easily interpreted using, e.g., a tight-binding (TB) model and the first-order perturbation theory [1,6]. The difference in energy of the A and B excitons is an experimental signature of the VB spin-splitting [3].
SOC also affects the CB. Initially, theoreticians disregarded this effect mainly because it is, indeed, very insignificant in the MoS$_2$ material, which is the most-extensively studied TMDC. The situation was assumed to be pretty much the same for other monolayer TMDCs. In general, the magnitude of the spin-splitting of the CB was just 7–10% of the magnitude of the VB, except for MoS$_2$, where it was as low as 2%: see Table 3 in Ref. [3]. However, in the absolute values this contribution can be important at low temperatures and in samples that show a ballistic effect (when charge carriers travel a long distance without significant scattering). It is worth noting that the SOC at the K point is more sublime in the CB than in the VB. In the first approximation, in which only atomic orbitals of the $d_{z^2}$ metals are taken into account, SOC vanishes. However, DFT calculations suggest that there is a finite spin-splitting at the K point of the CB.

It turns out that it is possible to explain the SOC in the CB in terms of a competition between the two contributions [4-6]:

- the first-order contribution from chalcogene atoms, which have a small but finite weight [4, 8];
- the second-order contribution due to coupling with other bands [4-6], where the atomic orbitals $d_{xz}$ and $d_{yz}$ have large weights: see Fig. 3 in Ref. [3]. Because of this competition, spin-polarization of spin-split CB is different in MoX$_2$ and WX$_2$. The latest results have been derived using the Fleur code, which enables the value of $\langle s_z \rangle$ in a given band to be derived explicitly. It has been found that a spin-split CB with $\langle s_z \rangle > 0$ ($\langle s_z \rangle < 0$) has a higher (lower) energy in MoX$_2$, while the opposite is true for WX$_2$: see figures 2(a) and 2(b), where the CBs of MoSe$_2$ and WSe$_2$ are, respectively, shown.

![Figure 2. Spin polarization and dispersion of spin-split CB and VB in the vicinity of the K point obtained from DFT calculations. The arrows indicate the direction of an average spin magnitude (red- upward rotation, blue- downward rotation). (a) and (c) show results for MoX$_2$; (b) and (d) for WX$_2$. The plots are borrowed from Ref. [3].](image)

By contrast, as illustrated in figures 2(c) and (d), in the VB, the sign of $\langle s_z \rangle$ is the same for both MoX$_2$ and WX$_2$. Besides, figures 2(a) and 2(b) also suggest that the band with a smaller effective mass has a lower energy for MoX$_2$, which leads to the crossing of the bands resulting from splitting due to spin-orbital coupling in the vicinity of the K and -K points [4-6]. As far as WX$_2$ is concerned, the band of interest has a smaller effective mass and higher energy and, hence, there is no crossing of bands. (A peculiar feature of MoTe$_2$ is that while there is no crossing of spin-split bands along the $\Gamma$ - K direction, there is a crossing along the K - M direction).
Despite the said differences, there is spin-valley coupling in the CB analogous to the VB. In figure 2, we also introduced the designation $K_{\text{vb}}^s$ ($K_{\text{cb}}^s$) for a higher-(lower-) energy VB, as well as for the CB. In optical experiments, due to spin polarization of bands, the low-energy spin-resolved transition takes the form $K_{\text{vb}}^s \rightarrow K_{\text{cb}}^s$ for MoX$_2$ and $K_{\text{vb}}^s \rightarrow K_{\text{cb}}^s$ for WX$_2$. We note that most recently, the first ARPES spin-resolved measurement has been reported for a slab WSe$_2$ [3], which is likely to indicate the spin polarization of the VB spin, with splitting taking place in the vicinity of the K and -K points. Assuming that measurements predominantly probe into the upper layer [9] i.e., in essence, a monolayer sample, they are in agreement with the DFT calculations presented in this work.

The dispersion in the vicinity of the K and -K points is not purely parabolic [11]. This needs to be taken into account when fitting a band structure in order to obtain the effective masses and other parameters of the band. This can be seen from figures 2(b) and (c) of Ref. [3], in which a trigonal warp (TW) of the dispersion curve can clearly be seen in the vicinity of the K and -K points. The TW is more pronounced for the VB, compared to the CB. In a simplest first approximation, this fact can be accounted for using a cubic term in the dispersion relation.

Dispersion in each spin-split band in the VB and CB is described by the expression:

$$E_k(q) = \frac{h^2 q^2}{2m_{\text{eff}}} + 3C_{\beta\lambda} q^4 \cos(2\varphi_x),$$

(5)

where the wave-vector $q = (q_x, q_y)$ is measured from the K point, $\varphi_x = \arctan(q_y/q_x)$, $m_{\text{eff}}$ is the effective mass of the charge carrier in the given band, and $C_{\beta\lambda}$ is a parameter that describes the TW. The derivation of $E_k(q)$ based on a multi-band $k\cdot p$ model was proposed in Ref. [3]. A similar model was recently employed in Ref. [11].

5. K-P Hamiltonian

Below, we derive a relationship for an effective low-energy $k\cdot p$ Hamiltonian that describes bound dynamics of the VB and CB. This topic was briefly discussed in Ref. [5], with the results then generalized and complemented in Ref. [3]. When constructing a model that would adequately describe the most important features of dispersion of the VB and CB, we can employ a seven-band model proposed in Ref. [5] as a first approximation. This model was discussed in detail in Ref. [3]. The effective low-energy $k\cdot p$ Hamiltonian can be derived from the seven-band model by systematically eliminating all degrees of freedom except for those that correspond to the VB and CB.

In Ref. [3], terms up to the third order were retained in the non-diagonal binding elements of the initial seven-band model while the spin basis was defined in the form $\{|\Psi^{vb}, s\rangle, |\Psi^{cb}, s\rangle\}$, where $|\Psi^{vb}, s\rangle, |\Psi^{cb}, s\rangle$ are spin-free Bloch wave-functions of the VB and CB, $|\Psi^{p}, s\rangle = |\Psi^{b}\rangle \otimes |s\rangle$, \(b = \{vb, cb\}, s = \{\uparrow, \downarrow\}\) denote the spin degree of freedom.

An effective low-energy $k\cdot p$ Hamiltonian is a sum of the following terms:

$$H_{\text{eff}} = H^s + H_{50}^s + H_{3p}^s,$$

(6)

where the free electron Hamiltonian $H^s$ takes the form:

$$H^s = \frac{h^2 q^2}{2m_{\text{e}}} - 3C_{\beta\lambda} q^2 \cos^2(2\varphi_x) \otimes s_z,$$

(7)

$s_z$ is the spin Pauli matrix, $m_{\text{e}}$ is the free-electron mass, and the wave-vector $q = (q_x, q_y)$ is measured from the K or -K points. It should be noted that while in the literature dealing with GaAs the term $H^s$ is ordinarily neglected due to its effective mass in the material, for the present purposes, we will retain it. The Hamiltonian $H_{50}^s$, which describes spin-orbital splitting, contains diagonal and $q$-independent SOC contributions. The Hamiltonian is expressed as follows:

$$H_{50}^s = \begin{pmatrix}
\tau V_{\alpha s} s_z & 0 \\
0 & \tau V_{\alpha s} s_z
\end{pmatrix}.$$

(8)

It is easy to see that the Hamiltonian is diagonal in the spin space and proportional to the Pauli matrix $s_z$. The Hamiltonian $H_{50}^s$ describes spin splitting of the CB and VB, which occur due to the lack of inversion symmetry in monolayer TMDCs. Considering that $H_{50}^s$ is diagonal, it can also be
expressed in terms of eigenvalues \( s = \pm 1 \). In this work, we use two types of designation. In the present context, the index \( \tau = 1 \) \((\tau = -1)\) denotes the vicinities of the \( K \) and \(-K \) points. Whenever it is more convenient, we utilize a \( \tau \) matrix, which operates in the valley space. In the VB, the parameter \( \Delta_{vb} \) describes the SOC intensity, which always takes positive values. It has been noticed that the situation with the CB is more complicated \([4–6]\), because the DFT calculations show that for \( \text{MoX}_2 \), spin splitting bands cross each other in the vicinity of the \( K \) and \(-K \) point, meanwhile no crossings occur for \( \text{WX}_2 \). This can be explained by the fact that the sign of \( \Delta_{cb} \) is opposite for \( \text{MoX}_2 \) and \( \text{WX}_2 \).

And, finally, the \( \mathbf{K}\mathbf{-P} \) Hamiltonian \( H_{\mathbf{K}\mathbf{P}} \) in Eq. (6) is defined as

\[
H_{\mathbf{K}\mathbf{P}}^{s} = H_{\mathbf{vb}}^{s} + H_{\mathbf{cb}}^{s} + H_{\mathbf{K}\mathbf{P}}^{s},
\]

where

\[
e_{vb}, e_{cb} \text{ is the band boundary, } \gamma_{s,t}, \alpha_{s,t}, \eta_{s,t}, \beta_{s,t}, \omega_{s,t} \text{ are the material constants. In the general case, the material parameters that enter } H_{\mathbf{K}\mathbf{P}}^{s} \text{ are complex numbers. For } \tau = -1 \text{ (the vicinity of the } -K \text{ point), the parameters are complex-conjugate relative to } \tau = 1 \text{ (the vicinity of the } K \text{ point). Specific values of the material parameters for each } \text{MX}_2 \text{ material can be found in Ref. [3].}

6. Interaction of the electromagnetic field with electrons in graphene and TMDCs

Let us assume that a linearly polarized electromagnetic field falls normally on a monolayer TMDC (Fig. 3).

\[
q_{z} = q_{z} + i \tau q_{z}, \quad \phi_{q} = \arctan \left( \frac{q_{y}}{q_{x}} \right),
\]

where

\[
H_{\mathbf{K}\mathbf{P}}^{s} = \left( \frac{\Delta_{s}^{2} + \tau s \Delta_{s}^{2}}{2} \right) \gamma \left( \tau k_{z} - i k_{z} \right) - \left( \frac{\Delta_{s}^{2} + \Delta_{s}^{2}}{2} \right) \gamma \left( \tau k_{z} + i k_{z} \right).
\]

An unperturbed Hamiltonian that describes the material of interest may be given in the form \([4,12]\):

\[
W_{q} = \left( \frac{\Delta_{s}^{2} + \tau s \Delta_{s}^{2}}{2} \right) \gamma \left( \tau k_{z} - i k_{z} \right) - \left( \frac{\Delta_{s}^{2} + \Delta_{s}^{2}}{2} \right) \gamma \left( \tau k_{z} + i k_{z} \right).
\]

Figure 3. Interaction of an electromagnetic field with a monolayer TMDC.
where \( k = (k_x, i k_y) \) is the electron wave-vector in the layer plane, \( \Delta \) is the band gap width, \( \gamma \) is proportional to the velocity of Fermi quasiparticles, \( \Delta^+ \) and \( \Delta^- \) are spin-orbital splittings of the VB and CB, respectively, \( s = \pm 1 \) is the spin index, and \( \tau = \pm 1 \) is the valley index, respectively, for the \( K \) and \( K' \). Hereafter, we analyze a monolayer found in the plane \((x, y)\) at \( z = 0 \). The interaction with the electromagnetic field is given by

\[
p \to p - eA(t),
\]

It is worth noting that all processes are handled here within a 'semi-classical quantum' theory, with the electromagnetic radiation being described in terms of classical electrodynamics and an electron subsystem treated in terms of non-relativistic quantum mechanics.

The Hamiltonian that involves the electromagnetic interaction takes the form [12]:

\[
W(k) = \begin{pmatrix}
0 & \frac{|e| \gamma (\tau \Delta_k - i \Delta_s)}{\hbar} \\
\frac{|e| \gamma (\tau \Delta_k + i \Delta_s)}{\hbar} & 0
\end{pmatrix} + \begin{pmatrix}
E^+_s & \gamma (\tau k_s - i k_y) \\
\gamma (\tau k_s + i k_y) & E^-_s
\end{pmatrix}.
\]

Let us analyze a linearly polarized incident field. If the field is polarized along the \( x \)-axis, the vector potential of the electromagnetic field takes the form:

\[
A^{ext}(x, y, t) = E_{ext} \cos \omega t \hat{x}.
\]

The Hamiltonian is given by

\[
W_0 = \begin{pmatrix}
0 & \Omega \tau \hbar \omega \\
\Omega \tau \hbar \omega & 0
\end{pmatrix} \cos \omega t.
\]

The interaction of the electromagnetic field with electrons is described by a free-electron Hamiltonian in a Dirac material [4]:

\[
W_k = \begin{pmatrix}
\Delta_k + \frac{\tau s \Delta^+_s}{2} & \gamma (\tau k_x - i k_y) \\
\gamma (\tau k_x + i k_y) & -\Delta_k - \frac{\tau s \Delta^-_s}{2}
\end{pmatrix}.
\]

The intensity of the field-electron interaction is described by the parameter

\[
\Omega = \frac{2|e| |E_{ext}|}{(\hbar \omega)^2}.
\]

To solve the equation, we shall use the solution of a non-stationary Schroedinger equation for the Hamiltonian:

\[
i \hbar \frac{\partial \psi_0}{\partial t} = W_0 \psi_0,
\]

The solution of this Hamiltonian is given by

\[
\psi_0 = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ \pm 1 \end{pmatrix} \exp \left[ i \frac{m \Omega \tau \sin \omega t}{2} \right].
\]

With these two solutions forming a basis, the solution of the general problem can be represented as a linear combination of basis solutions:

\[
\psi_k = a_1(t) \psi_0 + a_2(t) \psi_0.
\]

Then, substituting this solution into a non-stationary Schroedinger equation, we obtain an equation relative to the functions \( a_1(t), a_2(t) \) [12]:

\[
\]
From the Flocke theorem, the wave function takes the form:
\[
\Psi(t) = e^{-i\mathcal{H}_{\text{pot}}t} \phi(t).
\] (28)

We note that the quasi-energy of systems acted upon by a periodic perturbation has the same meaning as a conventional energy of stationary systems. These quantities define the energy spectrum of the electrons dressed by an electromagnetic field.

The periodicity of the function implies that
\[
\cos(n \omega t) \approx e^{-i\omega t}.
\] (29)

Substituting this expression into the original equation and applying an Anger-Jacobi expansion to the Bessel functions
\[
e^{i\omega t} = \sum_{n=-\infty}^{\infty} J_n(\omega) e^{in\omega t},
\] (30)
yields a time-independent set of equations:
\[
\sum_{n=-\infty}^{\infty} \sum_{j=1}^{2} W_{n,j}^{(j)} a_{n,j} = \tilde{E}(k) a_{n,j},
\] (31)

The matrix elements of a stationary Hamiltonian take the form [12]:
\[
W_{n,j}^{(j)} = \frac{E_{n,j} - E_{n,j}^*}{2} + i\gamma k_j \delta_{n,j},
\] (32)

The Hamiltonian takes the form [4]:
\[
W_{n,j}^{(j)} = \frac{E_{n,j} + E_{n,j}^* + \gamma \tau k_j + nh\omega}{2} \delta_{n,j},
\] (33)

The major contribution comes only from the terms with \(n=0\), which describe an elastic interaction between the electrons and the electromagnetic field. Neglecting minor terms, we find that in this approximation the solution of the Schrödinger equation takes a simple form:
\[
\sum_{j=1}^{2} W_{0,j}^{(j)} a_{0,j} = \tilde{E}(k) a_{0,j},
\] (34)

Using an unitary transform, the Hamiltonian can be reduced to
\[
\hat{H}_{\text{eff}}(k) = \begin{pmatrix}
\Delta_x/2 + \tau z \Delta_{\omega}^z/2 & \tau \gamma x k_x - i \gamma y k_y \\
\tau \gamma x k_x + i \gamma y k_y & -\Delta_y/2 - \tau z \Delta_{\omega}^z/2
\end{pmatrix},
\] (35)
The dispersion equation (quasi-impulse-dependence of energy) takes the form:

\begin{align}
\tilde{\varepsilon}_k &= \lambda_{\text{imp}} J_0(\Omega), \\
\tilde{\lambda}_{\text{cov}} &= \frac{2 \Delta_{\text{cov}} - \Delta_{\text{co}}}{2} + \frac{\Delta_{\text{cov}} + \Delta_{\text{co}}}{2} J_0(\Omega), \\
\tilde{\lambda}_{\text{c}} &= \frac{2 \Delta_{\text{c}} - \Delta_{\text{co}}}{2} + \frac{\Delta_{\text{c}} + \Delta_{\text{co}}}{2} J_0(\Omega).
\end{align}

(37) \hspace{2cm} (38) \hspace{2cm} (39)

The above-derived equation coincides with the equation derived in Ref. [12] in the strong-field approximation. It is worth noting that the Hamiltonian of a system interacting with the electromagnetic field is similar to the Hamiltonian of a free system up to designations:

\begin{align}
H_{\text{el}} \rightarrow H_{\text{el}}, \quad \Delta_{\text{cov}} \rightarrow \tilde{\Delta}_{\text{cov}}, \quad \tilde{\gamma}_{x,y} \rightarrow \tilde{\gamma}_{x,y}.
\end{align}

(41)

Hence, the dynamics of an electromagnetic-field-dressed electron is similar to that of a free electron. It should be noted that this result has been obtained as an approximation. The term 'strong electromagnetic field' means that the energy of photons in the incident field is much higher than the band gap width in the original material. The formulae derived above are well-suited for calculating the spectrum of charge carriers in the electromagnetic field when dealing with both graphene and TMDs.

As distinct from Ref. [12], in this work, the spectrum of the charge carriers was analyzed based on the solution of a set of equations

\begin{align}
\sum_{n_{\text{el}}} \sum_{j=1}^2 W_{nj}^{\eta,j} a_{nj}^{\eta,j} = \tilde{E}(k) a_{nj}^{\eta,j},
\end{align}

(42)

The solution of the set of equations is reduced to a problem of minimization of the determinant:

\begin{align}
\det \left( H_{nj}^{\eta,j} - \tilde{E}(k) \delta_{nj}^{\eta,j} \right) \rightarrow 0
\end{align}

The matrix \( M_{nj}^{\eta,j} = H_{nj}^{\eta,j} - \tilde{E}(k) \delta_{nj}^{\eta,j} \) is brought to a diagonal form before minimizing its minimal eigenvalue. This technique makes the algorithm more robust compared to when letting the matrix determinant tend to zero in a straightforward way. We have shown that for the parameters of Ref. [12], the calculation of \( \tilde{e}(k) \) gives a 2% difference. This serves to confirm a hypothesis set out in Ref. [12], stating that the major contribution to the interaction of electrons with the electromagnetic field comes from the terms with \( n=0 \), which describe the elastic interaction of an electron with an electromagnetic field.

7. Conclusion

In conclusion, it should be noted that the approach proposed in this work can be extended to other types of polarization of the electromagnetic field, such as circular, elliptic, and longitudinal polarization [13-14]. For the longitudinal polarization, the motion of charge carriers in the perpendicular direction to the plane of the two-dimensional material will need to be taken into account. In this work, the formulae were obtained in a strong field approximation, when the energy of photons is much higher than the band gap width. However, to conduct experimental observations, super-high incident energies need to be utilized. Such radiation is able to melt down the sample.

It would be of special interest to look into the behavior of charge carriers if the energy of photons in the illuminating beam becomes comparable with the band gap width. Although in this case the result is less elegant, it may give an instrument for controlling parameters of the materials with the aid of a weaker electromagnetic field. In the future, we plan to make an attempt to describe the interaction of 'non-classical' light with TMD.

8. References

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**Acknowledgements**

In this work, the analytical formulae were derived under the financial support of the RF Ministry of Science and Higher Education within a government contract of the FSRC for "Crystallography and Photonics", RAS (agreement 007-G3/43363/26) and the calculation of the diffraction orders of a hyperspectrometer grating was funded under the Russian Foundation for Basic Research grants ## 16-29-11744 and 16-29-09528.