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Excitations of Quasi-Two-Dimensional Electron Systems in Magnetic Field

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Introduction

Though quasi-two-dimensional systems had always been in the core of scientific interest, the first isolation of graphene, a two-dimensional carbon allotrope, in 2005 gave new impetus to the research of two-dimensional (2D) materials, [17], [22]. The peculiarity of graphene is rooted in its 2D nature, and manifests itself in extraordinary properties such as the conical band structure at low energies, or the unconventional quantum Hall effect, [5], [6]. The conical valleys, commonly referred to as Dirac cones, are described by the Dirac equation of massless particles, albeit with a much lower velocity v_F instead of the speed of light c. This property makes graphene the first 2D condensed matter system that hosts massless, charged fermions.

The boost in graphene's research is primarily engined by the fascination that the truly 2D nature of the material envoked, leading to the isolation and investigation of a plethora of other 2D materials as a direct consequence. A notable class is the transition metal dichalcogenides, prominant examples include MoS_2, $MoSe_2$, WS_2 or WSe_2, for details see Ref. [21]. Other noteworthy materials are hexagonal boron-nitride, germanene, silicon carbide or silicene. For a panoramic view of the properties of currently investigated 2D materials see [14]. Looking at the above list, it is clear that in spite of their common 2D nature these materials vary considerably as far as their electrical properties or band structure are concerned. Undeniably, such a versatility makes the 2D material research a cutting-edge research field.

Besides, the interest in graphene is also inspired by the presence of Dirac electrons, which induced a quest for such systems where the Dirac cones appear in the vicinity of the Fermi energy. In some three-dimensional layered organic compounds, including α-(BEDT-TTF)$_2$I$_3$ (aI3), the low-energy band structure is described by conical valleys. These crystals have strong 2D nature and massless fermions usually appear under high pressure or strain, [16], [18], [19].

However impressive the above list of quasi-2D materials may be, we should notice that the research of these materials is still intense with several open questions to be answered. Undoubtedly, graphene is the best known among them, though our understanding is not complete in this case either, [2], [11]. The same is particularly true for the other materials. For these reasons we believe that the theoretical investigation of the elementary properties and many-body effects of quasi-2D materials is a timely issue and reckons on general interest.

Goals and Methods

In the present thesis we will examine single-particle and collective excitations of quasi-2D materials including monolayer and bilayer graphene and layered organic crystal aI3. Our theoretical investigations will exclusively focus on properties in a strong magnetic field, where integer quantum Hall or quantum Hall ferromagnetic states appear.

The aI3 is particularly interesting for us, as its Dirac cones are anisotropic and tilted, in contrast to those of graphene, though the parameters describing the tilt and anisotropy have not been determined experimentally yet, only theoretical predictions exist, [7], [9], [10]. Here we aim to propose a suitable experimental procedure to measure these parameters. While determining the magneto-optical properties in a single-particle picture in Chap. 3, we find the emergence of a plethora of new transitions compared to the isotropic, non-tilted case. This yields a unique oscillation of the high-energy tail of the absorption coefficient, which may lead to the requested values of the parameters.

Moreover, besides the exact value of the Dirac cone parameters, the presence of a massive valley in the low-energy band structure is also a debated issue, [1], [15], [20]. Indeed, further experimental verification of the presence or absence of the massive valley is highly desired. By examining the PHES and calculating the density-density response function in Chap. 4, we intend to show that the response of the massive and the linear valleys is clearly distinguishable if we tune the magnetic field and/or by doping. Our predictions may contribute effectively to the precise determination of the low-energy band structure of the material.

In the case of bilayer graphene, the investigation of the interaction effects is a timely issue, as they turn out to be strong in this material. In Chap. 5 we calculate the dispersion relation of elementary excitations, which are magnetoexcitons, [3], [4], [8], [12], [13], in a mean-field approach, with the intention to show how Coulomb interaction modifies the dispersion relation in comparison with the single-particle picture. We find that the mixing of different Landau level transitions not only renormalizes the magnetoexciton modes, but essentially changes their spectra both at zero and finite wave vectors, and it also modifies the orbital character of the modes at finite wave vectors.

New Scientific Results

1. I have solved the eigenvalue problem of α-(BEDT-TTF)$_2$I$_3$ in a perpendicular magnetic field making use of the relativistic covariant nature of the underlying Dirac equation, assuming the material is under high hydrostatic pressure or uniaxial strain, that is, the zero-gap state phase is realized. I have drawn a parallel between the zero-gap state phase of α-(BEDT-TTF)$_2$I$_3$ and graphene in a crossed magnetic and in-plane electric fields and I have pointed out that the electric field in the latter system and the tilt in the former one play essentially the same role, leading to identical Landau states in both systems [III].

2. Handling graphene in a crossed magnetic and electric fields and α-(BEDT-TTF)$_2$I$_3$ in a magnetic field together I have calculated the frequency dependence of the absorption coefficient. Considering circularly polarized light, I have determined the matrix elements and I have found that besides the dipolar optical transitions $\propto \delta_{|n|,|n|\pm 1}$, a plethora of other optical transitions are possible due to rotational symmetry breaking. I have analyzed the internal structure of the emerging novel transitions and I have demonstrated

using Fourier transformation that it leads to an oscillatory behaviour of the high-frequency tail of the absorption coefficient, which might be measurable in both systems. I have proposed a procedure to deduce experimental value for the tilt parameter β and the tilt direction θ_{tilt} in α-(BEDT-TTF)$_2$I$_3$ [III].

3. I have determined the collective excitations of α-(BEDT-TTF)$_2$I$_3$ in its zero-gap state phase in a perpendicular magnetic field within the random phase approximation. I have calculated the frequency-dependent dielectric function and the density-density response function assuming the presence of both massive and massless carriers in the low-energy band structure. I have identified the linear magnetoplasmons of the linear and the upper-hybrid modes of both types of valleys and discussed their angular dependence. I have demonstrated that by magnetic field and doping one can tune the system between a case where only the linear valleys contribute to the density-density response and a case where all three valleys contribute. I have discovered that in an electron-doped case the angular dependence leads to a unique, anisotropic damping between the valleys: the particle-hole excitations of one valley damp the plas-

monic mode of the other valley, even though the latter is in its proper forbidden region. I have pointed out that in a hole-doped case the massive band dominates the collective excitations of the system, and it also participates in the damping processes among the valleys. I have analyzed how doping can effectively tune the system between isotropic and anisotropic screening regimes [II].

4. I have calculated the magnetoexciton dispersion relation of bilayer graphene in a perpendicular magnetic field in a mean-field picture. I have identified three terms that appear besides the single-body energy difference: first, the exchange self-energy difference of the two states involved, second, the direct dynamical interaction between the electron and the hole and, finally, the exchange interaction between the electron and the hole. I have enumerated the possible magnetoexcitons both in the integer quantum Hall regime, where the highest Landau level is fully filled, and in cases with other integer filling factors that correspond to symmetry-breaking quantum Hall ferromagnetic states. I have demonstrated that the cyclotron resonance is modified considerably by the inclusion of the Coulomb interaction both in the $k \to 0$ limit, as Kohn's theorem does not apply

in the case of bilayer graphene, and at finite wave vector. I have also pointed out that Landau level mixing leads to the elimination of level crossings, and that the mixing of transitions is especially strong in the intermediate k range, which is accessible experimentally by inelastic light scattering [I].

List of Publications

1. Publications related to the thesis

Publications in peer-reviewed journals:

[I] J. Sári and C. Tőke, Phys. Rev. B **87**, 085432 (2013).

[II] J. Sári, C. Tőke, and M. O. Goerbig, Phys. Rev. B **90**, 155446 (2014).

[III] J. Sári, M. O. Goerbig, and C. Tőke, Phys. Rev. B **92**, 035306 (2015).

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