A Dirac electron [1–3] moving in a rotationally invariant, localized and smoothly varying potential \( V(r) \) is described by the Hamiltonian

\[
H = \frac{p^2}{2m_e} + \frac{e}{c} A \cdot \mathbf{r} + V(r),
\]

where \( \mathbf{r} = (\sigma_x, \sigma_y) \) and \( \sigma_z \) are Pauli spin matrices (\( \mathbf{p} \) is the two-dimensional momentum). The shape of \( V(r) \) can be parabolic, Coulomb and Gaussian. Half-integer angular momentum \( J = \pm \frac{1}{2}, \pm \frac{3}{2}, \cdots \) is a good quantum number and wavefunctions of eigenstates have the form

\[
\chi_J(r) = \begin{pmatrix} \chi_A(r) e^{i(J-\frac{1}{2})\theta} \\ \chi_B(r) e^{i(J+\frac{1}{2})\theta} \end{pmatrix},
\]

where \( J = \pm \frac{1}{2} \) and \( J + \frac{1}{2} \), respectively. The half-integer angular momentum quantum numbers have values \( J = \pm \frac{1}{2}, \pm \frac{3}{2}, \cdots \). The Hamiltonian has several unusual features not present in the case of massive electrons. A simple scaling analysis [4] suggests that a localized potential \( V(r) \) can act as a strong perturbation and that it can be even more singular in graphene than in ordinary two-dimensional systems of massive electrons: the kinetic term of Dirac Hamiltonian scales as \( 1/r \) while the potential term scales as \( 1/r^2 \) and \( 1/r^3 \) for Coulomb and Gaussian short-range potentials, respectively. The other unusual feature is the presence of quasibound states with complex energies [5, 6].

These effects show up differently in a magnetic field \( B \) applied perpendicular to the two-dimensional plane (the vector

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It consists of A sublattice and B sublattice radial wavefunctions \( \chi_A(r) \) and \( \chi_B(r) \) with channel angular momenta \( J - \frac{1}{2} \) and \( J + \frac{1}{2} \), respectively. The half-integer angular momentum quantum numbers have values \( J = \pm \frac{1}{2}, \pm \frac{3}{2}, \cdots \). The Hamiltonian has several unusual features not present in the case of massive electrons. A simple scaling analysis [4] suggests that a localized potential \( V(r) \) can act as a strong perturbation and that it can be even more singular in graphene than in ordinary two-dimensional systems of massive electrons: the kinetic term of Dirac Hamiltonian scales as \( 1/r \) while the potential term scales as \( 1/r^2 \) and \( 1/r^3 \) for Coulomb and Gaussian short-range potentials, respectively. The other unusual feature is the presence of quasibound states with complex energies [5, 6].
In the absence of \( V(r) \) eigenenergies form degenerate Landau level (LL) energies while they split into discrete energies when \( V(r) \) is present, see figure 1. They can form true boundstates with real energies [6–8] in contrast to the case of no magnetic field. Moreover, in addition to the magnetic length, \( \ell = 25.66(B[T])^{-1/2} [\text{nm}] \), a new length scale \( R \) is introduced in the wavefunction: boundstates with a \( s \)-channel angular momentum component can become anomalous and develop a sharp peak of a width \( \ell \) inside the potential and a broad peak of size magnetic length \( \ell \) outside the potential [9]. Although the effect of the potential is strong it is partly mitigated by Klein tunneling and there is a competition between the two length scales \( R \) and \( \ell \): the peak is strong in the regime \( R \ell < 1 \), but small in the regime \( R \ell > 1 \) (in the limit \( R \ell \to 0 \) it diverges). These states are present in various potentials: regularized Coulomb [10, 11], parabolic [6, 12] and finite-range potentials [7, 9], see figures 2(a)–(c).

However, experimentally it is unclear how to probe these anomalous states. We propose in this paper that they can lead to positively s-enhanced optical conductivity and develop a sharp peak of a width \( \ell \). (a) Regularized Coulomb potential, (b) parabolic potential and (c) Gaussian potential. Horizontal lines indicate the energy levels. (d) Energy splitting of \( n = 0 \) (chiral) and 1 (nonchiral) LLs is shown. Filled squares represent occupied \( n = 0 \) LL states and open circles represent empty \( n = 1 \) LL states. Symbol A stands for an anomalous state. Arrows indicate optical transitions.

Coulomb interaction [16] may also affect these transitions. The energy scale of the interaction is significant in graphene at all values of magnetic fields \( B \) and each optically excited state is expected to be a correlated many-body state, containing a linear combination of several electron-hole pair states. This effect may change the value of the optical strength. We have investigated this issue for a completely filled LL by computing many-body correlated states within TDHFA [17–21] and have calculated the optical conductivity. In contrast to the naive expectation, we find that an excited electron-hole pair originating from the optical transition between two anomalous impurity states (see figure 2) is nearly uncorrelated with other electron-hole states, despite displaying substantial exchange self-energy effects. This absence of correlation is a consequence of a small vector correction in comparison to the difference between renormalized transition energies computed within the one electron-hole pair approximation. Many-body interactions do not enhance the strength of the optical conductivity of this transition. However, an excited electron-hole pair originating from the optical transition between a normal and an anomalous impurity states (see figure 2) can be substantially correlated with other electron-hole pairs with a significant optical strength.

This paper is organized as follows. In section 2 the optical matrix element of anomalous states is shown to be small using an idealized impurity model. The many-body version of the Kubo

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5 In the case of the impurity Coulomb potential a regularization parameter \( R \) must be introduced: \( V(r) = -\frac{e^2}{4\pi \varepsilon R} \) for \( r < R \) and \( \frac{e^2}{4\pi \varepsilon R} \) for \( r > R \) (\( \varepsilon \) is the dielectric constant). When the strength of the potential is strong this is needed to prevent the spurious effect of Coulomb fall to the center of the potential.

6 The natural length scale of a parabolic potential \( \frac{1}{2}\ell R^2 \) is \( R = \left( \frac{\hbar v_F}{k} \right)^{1/3} \).

7 Optical properties of bulk graphene at \( B = 0 \) have been investigated using various many-body techniques.

8 The dimensionless strength of the electron–electron Coulomb interaction is given by the ratio between the energy scales for the Coulomb interaction and LL energy separation \( \frac{e^2}{\varepsilon R} \) and note that this dimensionless coupling constant is independent of magnetic field. Hereafter we will set \( g = 0.5 \).
formula of optical conductivity is given in section 3. How the self-energy correction of a singly occupied LL state affects the optical conductivity is evaluated in section 4. In section 5 we investigate how important vertex corrections are for a completely filled LL. The final section 6 includes a summary and discussion.

2. Model potential: optical matrix elements of anomalous states

In order to compute the optical conductivity of anomalous states accurately we first solve exactly the single impurity problem and apply the TDHFA using these solutions. A similar method was used for massive electrons confined in a quantum dot [21]. We study optical properties of anomalous states using a simple model potential. We choose a cylindrical impurity potential [7] since its eigenstates and eigenvalues can be solved exactly in the presence of a magnetic field. This potential captures essential features of anomalous states of parabolic, Coulomb and Gaussian potentials. The potential has the shape

\[
V_J(r) = \begin{cases} 
V_I & r < R, \\
0 & r > R'.
\end{cases}
\]  (3)

where \(V_I\) is the strength of the potential and \(R\) is the radius of the cylinder. According to equation (2) the impurity state \(|n, J\rangle\) of \(n\)th LL with conserved angular momentum quantum number \(J\) has the following form of wavefunction \(\Psi_n^J(r)\)

\[
|\Psi_n^J(r)\rangle = \begin{pmatrix} \chi_{0,n}^J(r) e^{i(J-1/2)\phi} \\
\chi_{1,n}^J(r) e^{i(J+1/2)\phi} \end{pmatrix}.
\]  (4)

where the A-component has orbital angular momentum \(l_A = J - 1/2\) and B-component \(l_B = J + 1/2\). The radial wavefunctions are given in [7, 22].

In reference [21], just like in our approach, the states of a quantum-dot in a magnetic field are obtained exactly before applying Hartree–Fock method.

In the absence of a potential these functions are related to Laguerre polynomials.

\[
\Psi_n^J(r) \sim e^{-br} r^{\Delta J}, \quad r > R
\]

where the sublattice index \(\sigma = A, B\) and \(U(x, y, z)\) and \(M(x, y, z)\) are confluent hypergeometric functions. The impurity eigenenergy is denoted by \(E_{n,j}\) and is plotted as a function of \(J\) for LL indices \(n = 0\) and 1 in figure 2(d).

Let us investigate which impurity states \(\Psi_n^J(r)\) can be anomalous, i.e. which of these states can have s-wave radial functions. It is possible only for states with \(J = \pm 1/2\), see equation (2). Using confluent hypergeometric functions and equation (4) it can be shown that, for \(n = 0\) LL, only the state \(\Psi_{0}^{-1/2}(r)\) has value at the origin \(\Psi_{0}^{-1/2}(0) \neq 0\) since its the B-component radial wavefunction \(\chi_{0}^{0}(r)\) is s-wave. While, for \(n = 1\) LL, both \(\Psi_{1}^{-1/2}(r)\) and \(\Psi_{1}^{1/2}(r)\) can be anomalous since their B- and A-components of radial wavefunctions are s-wave, respectively. These states are labeled by \(A\) in figure 2(d). They actually become anomalous when the condition \(R/\ell < 1\) is satisfied, see figure 3.

Phons are assumed to be polarized along \(x\)-axis and the optical matrix elements can be computed using the current operator \(j = \text{e}_x \sigma\). They satisfy the selection rules with the change of LL index \(\Delta n = 1\) and change of angular momentum \(\Delta J = 1\) and the relevant single-particle optical transitions are of the type \([0, J] \rightarrow [1, J + 1]\). The optical matrix element between the relevant anomalous states can be expressed in terms of the corresponding radial wavefunctions (see equation (4))

\[
\langle 1, 1/2| e^{i\theta}\chi_{1,B}^0 e^{-i\theta}\chi_{0,A}^1 + \langle 1, 0| e^{i\theta}\chi_{1,B}^0 \rangle e^{-i\theta}\langle 0, 0| \rangle
\]  (6)

In order to understand why this optical matrix element can be small the radial wavefunctions \(\chi_{1,A}^0(r)\) and \(\chi_{0,B}^0(r)\) in \(\chi_{1,B}^0\)

11 In the presence of a strong impurity potential the selection rule \(\Delta n = 1\) must be relaxed since different LLs get mixed. However, the corresponding transitions have small matrix elements and will be ignored in the following.
are plotted, together with the integrand of \( \int dr r_{\gamma \alpha}(r)^s \chi_{0,0}^0(r) \), in figure 3. We see from the shape integrand, figures 3(b)–(d), that the resulting integral is smaller than the corresponding integral in the absence of the localized potential plotted in figure 3(a). The actual values of transition matrix elements \( \langle 1, J|\sigma J |0, J \rangle \rangle^2 \) are given in table 1 for varies values of \( \langle V/ E_M, R/l \rangle (J, J') \).

The dependence of the transition matrix elements on the parameters \( \langle V/ E_M, R/l \rangle \) is non-trivial. Note that they depend significantly on the ratio \( RL/l \), i.e. on the magnetic field.

### 3. Optical conductivity

We compute the many-body optical conductivity in the presence of a single impurity (when more impurities are present in the dilute limit the total optical conductivity is given by the sum of the optical conductivity of each impurity [23]). We consider excitations from a singly occupied LL or completely filled LL (partially filled LLs cannot be described adequately in TDHFA since screening becomes important). The groundstate is denoted by \( |\psi_0 \rangle \) and it represents either a singly occupied LL or completely filled LL. In this case the optical conductivity consists of a series of discrete peaks.

Generally a many-body excited state can be written as a linear combination of single-electron excited states

\[
|\psi \rangle = \sum_J C_J |\psi_J \rangle, \tag{7}
\]

where single-electron excited states with \( \Delta J = 1 \) are

\[
|\psi_J \rangle = a^{\dagger}_{n, J+1} a_{n, J} |\psi_F \rangle. \tag{8}
\]

Here the operator \( a_{n, J}^{\dagger} \) creates an electron in the localized state of \( n \)th LL with angular momentum \( J \). The optical conductivity consists of a series of discrete peaks at the renormalized excitation energies \( E_{ex} \)

\[
\sigma(E) = \sum_{E_{ex}} \delta(E - E_{ex}), \tag{9}
\]

where \( s(E) \) is the optical strength. When this strength is divided by a constant \( c = 1/(\sqrt{2} E_M) \) it has a dimension of conductivity (if another value of \( c \) is chosen the magnitude of this scaled conductivity will be different). The scaled optical strength is computed using the Kubo formula

\[
\tilde{s}(E_{ex}) = \frac{s(E_{ex})}{1/(\sqrt{2} E_M)} = \frac{\pi e^2}{2 \hbar} \langle |\psi | T |\psi_F \rangle \langle \psi_F | T |\psi \rangle. \tag{10}
\]

### Table 1. Transition matrix elements \( \langle 1, J|\sigma J |0, J \rangle \rangle^2 \).

| \( (V/ E_M, R/l)(J, J') \) | \( 1/2 \) | \(-1/2 \) | \(-1/2 \) | \(-3/2 \) | \(-5/2 \) | \(-7/2 \) | \(-9/2 \) |
|-----------------|--------|--------|--------|--------|--------|--------|--------|
| (−2, 1)         | 0.137  | 0.263  | 0.377  | 0.487  | 0.5    |        |        |
| (−2, 0.3)       | 0.025  | 0.146  | 0.5    | 0.5    | 0.5    |        |        |
| (−20, 0.1)      | 0.157  | 0.341  | 0.5    | 0.5    | 0.5    |        |        |

### 4. Singly occupied Landau level

Before we investigate the effect of many-body correlations on the optical conductivity of anomalous states we compute it without them and include only self-energy effects. This calculation is a good approximation and is experimentally relevant when the \( n = 0 \) LL is occupied by only one electron. In this case only one term survives in the linear combination divided by constant \( c = 1/(\sqrt{2} E_M) \) it has a dimension of conductivity (if another value of \( c \) is chosen the magnitude of this scaled conductivity will be different). The scaled optical strength is computed using the Kubo formula

\[
\tilde{s}(E_{ex}) = \frac{s(E_{ex})}{1/(\sqrt{2} E_M)} = \frac{\pi e^2}{2 \hbar} \langle |\psi | T |\psi_F \rangle \langle \psi_F | T |\psi \rangle. \tag{10}
\]

where the scaled excitation energy is \( \tilde{E}_{ex} = E_{ex}/(\sqrt{2} E_M) \). When photons are polarized along the \( x \)-axis the optical matrix element is given by \( \langle \Psi | T |\psi \rangle \), where

\[
T = \sum_J \langle \psi_J + 1 |\sigma J |0, J \rangle a_{n, J+1}^{\dagger} a_{n, J} + h. c. \tag{11}
\]

The computed optical matrix element for \( n = 0 \) and \( n' = 1 \) LLs can be written in terms of expansion coefficients \( C_J \) and the optical many-body matrix elements

\[
\langle \Psi | T |\psi_F \rangle = C_{1/2} \langle 1, 1/2 |\sigma J |0, 1/2 \rangle + C_{3/2} \langle 1, 3/2 |\sigma J |0, 3/2 \rangle + C_{5/2} \langle 1, 5/2 |\sigma J |0, 5/2 \rangle + C_{7/2} \langle 1, 7/2 |\sigma J |0, 7/2 \rangle + \ldots. \tag{12}
\]

### Figure 4. A single electron is in the \( n = 0 \) LL. The LLs \( n = -1, -2, \ldots \) are all filled.

where photons are polarized along the \( x \)-axis.
The Hartree self-energy originates from the electronic density andionic potential and has two parts

\[
\Sigma_{h,J}^{\alpha} = \begin{cases} 
\sum_{n,J} f_{n,J} \langle m, J; n', J'|V|m, J; n', J'\rangle \\
- \sum_{n,J} f_{n,J} \langle m, J; n', J'|V|m, J; n', J'\rangle
\end{cases}
\]

(14)

where electron–electron interaction is \(V(\mathbf{r}_1 - \mathbf{r}_2) = \frac{e^2}{\epsilon |\mathbf{r}_1 - \mathbf{r}_2|}\)

and the occupation functions \(f_{n,J} = 1/0\) if the \(|n,J\rangle\) state is occupied/unoccupied. The second term represents a correction due to uniform ionic potential \(\langle n, l |\) represents a LL state of graphene in the absence of an impurity potential). The Hartree self-energy corrections are negligibly small. The exchange self-energy is given by

\[
\Sigma_{m,J}^{\chi} = - \sum_{n,J} f_{n,J} \langle m, J; n', J'|V|m, J; n', J'\rangle
\]

(15)

when \(K\) and \(K'\) valleys are uncoupled \cite{24}. Energies corrected by these exchange self-energy corrections are shown in figure 5.

The scaled optical strength of equation (10) is given by

\[
\tilde{s}(E_{\text{ex}}) = \frac{\pi e^2}{\hbar} \left[11, J + 1|e_0[0,J]\right]^2 / E_{\text{ex}}
\]

(16)

where the scaled excitation energy is given by the difference between renormalized impurity energies \(E_{\text{ex}} = (E_{J,J+1} - E_{0,0})/(\sqrt{2} E_{M})\). The computed scaled optical strengths are shown in figure 6. Let us first discuss the results in the absence of self-energy corrections. When \((V/J)/E_{M}, R/l) = (-2, 1)\) the bare transition between anomalous states, \(n = 0 \rightarrow 1\) with \(J = -1/2 \rightarrow 1/2\), has a small optical matrix element \(|0, -1/2|\sigma_1[1, 1/2]\rangle^2 = 0.137\). The resulting value of the scaled optical strength is also small with the value 0.325 \(\pi e^2 / 4\hbar\) see figure 6(b). For other bare transitions the optical matrix elements are larger and their scaled optical strengths are bigger \(\frac{1}{2} \pi e^2 < \tilde{s}(E_{\text{ex}}) < \pi e^2 / 4\hbar\). A similar result also holds for \((V/J)/E_{M}, R/l) = (-7.9, 0.3)\), see figure 6(a). We see that the values of the scaled optical strength are almost unchanged by the exchange self-energy corrections (In figure 6 any two transitions labeled by same \(J\) have similar strength values). However, the corresponding renormalized excitation energies display significant changes from those of bare transitions.

5. A filled Landau level

When a LL is completely filled both many-body correlations and self energy effects may be important. Here we investigate how they may affect the optical conductivity of anomalous states. Here we assume that \(n = 0, -1, -2, ...\) LLSs are filled. An optical transition leaves a hole in the filled \(n = 0\) LL, see figure 7(a). Since there can be several electron-hole excitations with \(\Delta J = 1\) an eigenstate is given by a linear combination of these electron-hole states. This implies that many-body correlation effects may be important. In this section we evaluate the magnitude of the excitonic and depolarization many-body effects (they are depicted in figure 7(b)). Since \(n = 0\) LL is also filled in addition to the \(-1, -2, ...\) LLSs the exchange self-energy acquires an additional correction in comparison to the case of singly occupied \(n = 0\) LL. The new exchange self-energies are shown in figure 8. In this section we explore whether these features can affect the optical conductivity in a significant way.

5.1. Many-body Hamiltonian matrix

The electron-hole excitations form basis states of the Hamiltonian matrix. Some of these configuration states are
Despite the presence of mixing between different electron configurations, we find that the renormalized transition energy of \( |0, J \rangle \rightarrow |1, J + 1 \rangle \) can be computed approximately using a diagonal approximation: it is equal to \( E_d^f \), see equation (18) (to compute the values of optical strength accurately one may have to go beyond the diagonal approximation). It can be broken into various components.
transition energy is 1.46$E_M$, which is close to the renormalized value. So despite strong mixing the diagonal approximation gives a good estimate of transition energies.

5.3. Results of optical conductivity

Let us show the result of the optical conductivity obtained by including full many-body effects. We diagonalize 5 × 5 Hamiltonian matrices (here we are mostly interested in lower energy excitations than that of magnetoplasmons; a significantly larger Hamiltonian matrix is needed to describe magnetoplasmon physics). The many-body eigenstates are given by the linear combination of electron-hole pair states $|\psi\rangle$ (see equation (7)). The obtained result for the scaled optical strength, given by equation (10), is displayed in figure 12 together with the bare values in the absence of many-body effects.

A transition between two anomalous impurity states is labeled by $-1/2$, see figures 12(a) and (b). It is created by the transition between two impurity anomalous states $|0, -1/2\rangle$ and $|1, 1/2\rangle$, see figure 2. Our numerical work shows that it involves dominantly only one electron-hole pair state $|\psi\rangle$ labeled by a single value of $E_{\mathbf{k},\mathbf{p}}$ (see figure 12(b)). It is nearly uncorrelated, displaying a unique feature of the physics of finite magnetic fields. The anomalous boundstates are strongly localized inside the well with a broad peak outside the well with width comparable to the magnetic length. In this paper we have proposed that anomalous boundstates may exhibit an unusually small value of magneto-optical conductivity since optical matrix elements of anomalous states are negligible compared to those of ordinary states. The effect of many-body interactions on their optical conductivity is investigated for a completely filled LL using a self-consistent TDHFA. We find that an excited electron-hole state originating from the optical transition between two anomalous impurity states exhibits small correlations with other electron-hole states, despite displaying substantial exchange self-energy effects. This is a consequence of a small vertex correction in comparison to the difference between renormalized transition energies computed within the one electron-hole pair approximation. We find that many-body interactions do not enhance the strength of its optical conductivity. However, by tuning the value of the magnetic field its strength may be enhanced significantly. There is also a transition between a normal and an anomalous impurity state. Unlike the optical transition between two anomalous states, we find, in this case, that the optically created electron-hole pair can be substantially correlated with other electron-hole pairs and that its optical strength can be significant.

Note that the eigenenergies of a parabolic potential are complex, implying that the lifetime in the potential is finite. For optical studies states with a small imaginary part of the eigenenergies are desirable. If the confining potentials vary fast there may be some valley mixing, which leads to a splitting of eigenenergies [25]. A tight-binding calculation can be used to investigate this effect.

Recently several infrared absorption experiments of graphene have been performed [26–29]. We suggest that this type of experiment be performed in magnetic fields on donor impurities or on quantum dot arrays in graphene, just like the case of two-dimensional massive electrons [13, 14, 29]. It would be interesting to observe anomalous transitions in the impurity cyclotron resonance in the regime $R/\ell < 1$ and confirm the sensitive dependence of their optical strength on the magnetic
field. In this paper we have considered donor impurities. For acceptors or antidots [25] we can use the transformation $V(r) \rightarrow -V(r)$ with the eigenenergies $E \rightarrow -E$ (eigenstates are unchanged).

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