Solution of the X-ray edge problem for 2D electrons in a magnetic field

H. Westfahl Jr.\(^1\), A.O. Caldeira\(^1\), D. Baeriswyl\(^2\), and E. Miranda\(^1\)

\(^1\)Instituto de Física Gleb Wataghin
Universidade Estadual de Campinas
13083-970, Campinas, SP, Brazil
\(^2\)Institut de Physique Théorique
Université de Fribourg, Pérolles
CH-1700 Fribourg, Switzerland

(March 24, 2022)

The absorption and emission spectra of transitions between a localized level and a two-dimensional electron gas, subjected to a weak magnetic field, are calculated analytically. Adopting the Landau level bosonization technique developed in previous papers, we find an exact expression for the relative intensities of spectral lines. Their envelope function, governed by the interaction between the electron gas and the core hole, is reminiscent of the famous Fermi edge singularity, which is recovered in the limit of a vanishing magnetic field.

Optical absorption and emission processes from core states in metals are expected to show striking many-body effects close to the threshold energy. This so-called X-ray edge singularity is dominated by two competing effects. On the one hand by the Anderson orthogonality catastrophe\(^1\), leading to a strong reduction of intensity and, on the other hand, by the attractive electron-core-hole interaction, leading to the power law divergence at the X-ray absorption edge predicted by Mahan\(^2\).

A unified description of the two effects was first provided by Nozières and de Dominicis\(^3\) by treating the electron-core-hole interaction as a one-body scattering potential, switched on suddenly at the time of the X-transition. They found that the nature of this behavior - divergent or convergent - is controlled by the scattering phase shifts.

A particularly transparent analysis of the problem was subsequently given by Schotte and Schotte\(^4\) in terms of a bosonization scheme, inspired by previous work on the Tomonaga model\(^4\). On the one hand, the orthogonality catastrophe is viewed as a consequence of the infinite number of low energy electron-hole pairs generated in the vicinity of the Fermi surface (shake-up) due to the sudden appearance of the scattering potential. On the other hand, the Mahan effect is interpreted as a consequence of the interference between the bosons created in the shake-up and those representing the extra electron in the bosonization scheme.

The theoretical predictions appear to agree with X-ray spectra for the first five metallic elements of the periodic table, although the interpretation of the spectra is rendered difficult by possible band structure effects. Advances in the growth of modulation-doped semiconductor heterostructures have made it possible to investigate the same kind of processes in quasi-two-dimensional electron gases. In a pioneering work, Skolnick \textit{et al.}\(^5\) found evidence for a Fermi edge singularity in the low-temperature photoluminescence spectra of InGaAs-InP quantum wells. This is surprising since in interband transitions the hole recoil is expected to damp the edge singularity. Skolnick \textit{et al.} argued that the minority carriers are localized due to alloy fluctuations and thus behave like core holes in X-ray emission. This interpretation agrees with experiments on cleaner samples\(^6\) where the effect is considerably weaker.

The experiments were also carried out in the presence of a perpendicular magnetic field\(^7\) where the situation is drastically changed, since the conduction-band states are quantized into discrete Landau levels. In this case, the sudden appearance of the hole potential generates excitations, in which electrons are promoted from one Landau level to another, across the Fermi energy. As a result, both Mahan and Anderson phenomena show up in the relative intensities of the discrete emission peaks.\(^8\) A theory of optical and magneto-optical phenomena in quasi-two-dimensional electron gases was given in a series of papers by Hawrylak\(^9\) and Uenoyma and Sham\(^10\).

Inspired by the work of Schotte and Schotte\(^4\), we adopt a bosonization scheme to study the magneto-optical spectra of electronic transitions between a localized non-degenerate level and the Landau levels of a two-dimensional electron gas. This allows us to derive for the first time, to the best of our knowledge, an analytical expression for the relative intensities of the emission peaks.\(^11\) Our model is very similar to the one used in the study of core level absorption spectra in metals\(^12\) and in previous works on two-dimensional electron systems.\(^13\) The Hamiltonian consists of three contributions

\[
H = H_0^{(c)} + H_0^{(h)} + H_1^{(c-h)}.
\]

The first term describes independent electrons (taken here as spinless) of effective mass \(m\) in a magnetic field. For a disk geometry and the symmetric gauge, \(H_0^{(c)}\) can be diagonalized in terms of angular momentum eigenstates.\(^14\)

\[
H_0^{(c)} = \sum_{n=0}^{\infty} \sum_{m_z = -n}^{n} (n\omega_n - \mu)c_{nmz}^\dagger c_{nmz},
\]

where the situation is drastically changed, since the conduction-band states are quantized into discrete Landau levels. In this case, the sudden appearance of the hole potential generates excitations, in which electrons are promoted from one Landau level to another, across the Fermi energy. As a result, both Mahan and Anderson phenomena show up in the relative intensities of the discrete emission peaks.\(^8\) A theory of optical and magneto-optical phenomena in quasi-two-dimensional electron gases was given in a series of papers by Hawrylak\(^9\) and Uenoyma and Sham\(^10\).

Inspired by the work of Schotte and Schotte\(^4\), we adopt a bosonization scheme to study the magneto-optical spectra of electronic transitions between a localized non-degenerate level and the Landau levels of a two-dimensional electron gas. This allows us to derive for the first time, to the best of our knowledge, an analytical expression for the relative intensities of the emission peaks.\(^11\) Our model is very similar to the one used in the study of core level absorption spectra in metals\(^12\) and in previous works on two-dimensional electron systems.\(^13\) The Hamiltonian consists of three contributions

\[
H = H_0^{(c)} + H_0^{(h)} + H_1^{(c-h)}.
\]

The first term describes independent electrons (taken here as spinless) of effective mass \(m\) in a magnetic field. For a disk geometry and the symmetric gauge, \(H_0^{(c)}\) can be diagonalized in terms of angular momentum eigenstates.\(^14\)

\[
H_0^{(c)} = \sum_{n=0}^{\infty} \sum_{m_z = -n}^{n} (n\omega_n - \mu)c_{nmz}^\dagger c_{nmz},
\]
where \( c_{n,m_z} \) creates an electron in a Landau level \( n \) with azimuthal angular momentum \( \ell m_z \), \( \omega_c = e B / \hbar m_e \) is the cyclotron frequency, \( \mu \) is the chemical potential (including the zero point energy \( \hbar \omega_c / 2 \)) and \( N_\phi = \frac{2 S}{\phi_0} \) is the number of flux quanta \( \phi_0 \) piercing a sample of area \( S \).

The second term describes a localized hole and is written as

\[
H_0^{(h)} = \hbar \omega_0 d^\dagger d,
\]

where \( d^\dagger \) creates a hole in a non-degenerate level of energy \( -\hbar \omega_0 \) (measured from the chemical potential). Its wave function is assumed to be strongly localized at the origin and to have \( s \)-wave symmetry.

The third contribution refers to the electron-hole coupling, which we represent by a spherically symmetric potential. Angular momentum is therefore conserved and the potential scatters electrons from \( (n,m_z) \) to \( (n',m_z) \).

Following Schotte and Schotte we represent this coupling by a contact potential at the origin,

\[
H_I^{(e-h)} = V_0 \psi(0) \Delta(0) d^\dagger d,
\]

where \( \psi(0) = \sum_{n,m_z} \psi_{n,m_z}(0) c_{n,m_z} \) is the fermion field operator at \( r = 0 \). This simplifies considerably the analysis, since wave functions with \( m_z \neq 0 \) vanish at the origin, \( \psi_{n,m_z}(0) = \frac{e^{i m_z \phi}}{\sqrt{2 \pi m}} \delta \) (where \( \ell = \sqrt{2 \pi m} \omega_c \) is the magnetic length), and are therefore not affected by the localized hole. Then, defining \( \delta_B/\pi = -V_0 \rho_F \) with \( \rho_F = \frac{m}{2 \pi \hbar^2} \)

being the density of states for \( B = 0 \), we arrive at the simplified electron-hole interaction Hamiltonian

\[
H_I^{(e-h)} = -\hbar \omega_c \frac{\delta_B}{\pi} \sum_{n',n} c_{n',0}^\dagger c_{n,0} d^\dagger d.
\]

Analogously to the Schotte and Schotte paper, \( \delta_B \) can be identified as the phase shift in the Born approximation. We remark that the scheme developed in this paper can be easily generalized to the case of finite range spherically symmetric potentials.

For simplicity, we restrict ourselves to the case of a relatively weak magnetic field, tuned in such a way that the \( N \) electrons fill completely the \( \nu = N/N_\phi \) lowest Landau levels. This corresponds to an integer quantum Hall regime with large filling factor. Thus the ground state of \( H^{(e)}_0 \) is given by

\[
|G_0\rangle = \prod_{n=0}^{\nu-1} \prod_{m_z=-n}^{N_\phi-n} c_{n,m_z}^\dagger |0\rangle. \tag{1}
\]

At this point we adopt a Landau level bosonization scheme, introduced in previous papers to express all the excitations of the electronic system in terms of bosonic fields.

In a first step we enlarge the Hilbert space by including negative \( n \) states, in the spirit of the Luttinger model. Accordingly, the ground state \( |G_0\rangle \) has to be redefined, so that all the negative energy states are completely filled. These unphysical states should have little influence on the low-energy excitations.

Next we introduce the bosonic operators

\[
b_{n,m_z}^\dagger = \frac{1}{\sqrt{n}} \sum_{p=-\infty}^{\infty} c_{n+p,m_z,p,m_z}^\dagger \text{ for } n \geq 1,
\]

which generate neutral excitations above the ground state. In order to bosonize the fermion operators, we use the phase representation

\[
c_{n,m_z}^\dagger (\theta) = \frac{1}{\sqrt{2\pi \epsilon}} e^{i \theta} e^{i S_{n,m_z}^z (\theta)} c_{n,m_z}^\dagger.
\]

In close analogy to bosonization in one dimension, we express these operators in terms of bosonic fields,

\[
c_{n,m_z}^\dagger (\theta) = \frac{1}{\sqrt{2\pi \epsilon}} e^{i \theta} e^{i \Phi_{n,m_z}^z (\theta)} U_{n,m_z}.
\]

Here \( U_{n,m_z} \) is a unitary operator which increases the number of fermions with angular momentum \( m_z \) and provides us with the appropriate anticommutation properties. \( \Phi_{n,m_z}^z (\theta) \), defined for each angular momentum channel as

\[
\Phi_{n,m_z}^z (\theta) = N_{m_z} \theta - i \sum_{n=1}^{\infty} \frac{e^{-\mu \sqrt{n}}}{\sqrt{n}} \{ e^{i \theta} b_{n,m_z}^\dagger - e^{-i \theta} b_{n,m_z} \},
\]

is equivalent to the chiral phase operator of 1-D bosonization and \( N_{m_z} = \sum_p c_{p,m_z}^\dagger c_{p,m_z} - (c_{p,m_z}^\dagger c_{p,m_z}^\dagger) \) is the charge operator. Instead of taking the limit \( \epsilon \rightarrow 0 \), we can interpret \( 1/\epsilon \) as a bandwidth cutoff eliminating large \( n \) contributions. This cutoff increases as \( \nu \) increases, but the final result is cutoff independent, as in the solution of Schotte and Schotte.

The main difference to the bosonization introduced before is that here a channel is identified by its angular momentum instead of its guiding center. This choice is indeed more useful in the present case since all shake-up processes produced by the spherically symmetric potential conserve angular momentum.

We describe now emission and absorption processes due to transitions between the localized level and Landau levels. We assume the selection rule \( m_z = 0 \), which is justified if the hole wave function is spherically symmetric.

In the case of absorption the system is initially in the ground state \( |G_0\rangle \). Neglecting the \( n \)-dependence of the dipole matrix elements, we find a transition rate

\[
W_\alpha (\omega) \propto \sum_f \langle f | c_{0}^\dagger (0) | G_0 \rangle^2 \delta \left( \omega - \omega_0 + \frac{E_0 - E_f}{\hbar} \right),
\]

where the summation is performed over all states \( |f\rangle \) of the electron gas with one electron more than in the ground state \( |G_0\rangle \). The transition rate can be rewritten as
\[ W_a (\omega) \propto \text{Re} \int_0^\infty dt e^{i\omega t} F_a (t), \quad (3) \]

where

\[ F_a (t) = e^{-i\omega t} \langle G_0 | e^{iH_1 t/\hbar} c_0 (0)e^{-iH_1 t/\hbar} c_0^\dagger (0) | G_0 \rangle. \quad (4) \]

The initial and final Hamiltonians \( H_i \) and \( H_f \), respectively, can be represented in bosonized form. Since \( F_a (t) \) involves the propagation of zero angular momentum states, we can limit ourselves to

\[ H_i = \hbar \omega_c \sum_{n=1}^{\infty} nb_{n,0}^\dagger b_{n,0}, \]

for the Hamiltonian before the absorption (no hole) and

\[ H_f = \hbar \omega_c \sum_{n=1}^{\infty} \left\{ nb_{n,0}^\dagger b_{n,0} - \frac{\delta B}{\pi} \sqrt{n} \left( b_{n,0}^\dagger + b_{n,0} \right) \right\}, \]

for the Hamiltonian after the absorption (hole present).

Therefore, in terms of the bosons, the hole potential is a simple shift operator which generates the unitary transformation

\[ T = \exp \left[ \sum_{n=1}^{\infty} \frac{-\delta B}{\pi} \sqrt{n} \left( b_{n,0}^\dagger - b_{n,0} \right) \right]. \quad (5) \]

Apart from a constant term that does not affect the dynamics, the Hamiltonians \( H_f \) and \( H_i \) are connected through the relation \( H_f = TH_i T^\dagger \).

This simplifies the expression \( F_a \) to

\[ F_a (t) = e^{-i\omega t} \langle G_0 | a_0 (0, t)a_0^\dagger (0, 0) | G_0 \rangle, \]

where the new fermion operator \( a_{m_\theta} (\theta, t) \) is defined by

\[ a_{m_\theta} (\theta, t) = e^{iH_1 t/\hbar} c_{m_\theta} (\theta) T e^{-iH_1 t/\hbar}. \quad (6) \]

Therefore our task is to evaluate the correlation function of the operator \( a_0 (0, t) \) that simultaneously shifts the bosonic fields and creates an electron in a superposition of Landau levels with zero angular momentum. This can be easily done by using the bosonized version of the fermion operators, since the operator \( T \) is also an exponential of bosonic fields. Then, using equations \( F_a \) and \( F_c \), it is possible to show that

\[ F_a (t) = e^{-i\omega t} \frac{1}{2\pi \varepsilon} \langle G_0 | e^{-i\hat{\Theta}_0 (0,t)} e^{i\hat{\Theta}_0 (0,0)} | G_0 \rangle \]

\[ = e^{-i\omega t} \frac{1}{2\pi \varepsilon} e^{i \left( D_0 (0, t) - D_0 (0, 0) \right)}, \]

where

\[ D_0 (0, t) = \langle G_0 | \hat{\Theta}_0 (0, 0) | G_0 \rangle, \quad (7) \]

and \( \hat{\Theta}_0 (0, t) \) is written as

\[ \hat{\Theta}_0 (0, t) = -i \left( 1 - \frac{\delta B}{\pi} \right) \sum_{n=1}^{\infty} e^{-\frac{n\varepsilon}{\pi}} \left\{ e^{i\omega_c t} b_{n,0}^\dagger - h.c. \right\}. \quad (8) \]

After substituting the expression \( F_a \) into \( F_c \) we arrive at

\[ D_0 (0, t) - D_0 (0, 0) = (1 - \frac{\delta B}{\pi})^2 \ln \left( \frac{\varepsilon}{1 - e^{-i(\omega_c t - ie)}} \right), \]

that transforms the correlation function \( F_a \) into

\[ F_a (t) = \frac{e^{-i\omega t}}{2\pi \varepsilon} \left( \frac{\varepsilon}{1 - e^{-i(\omega_c t - ie)}} \right) \left( 1 - \frac{\delta B}{\pi} \right)^2. \]

Inserting this result into equation \( F_c \) we finally obtain the absorption spectrum

\[ W_a (\omega) \propto \sum_{\nu=1}^{\nu} \frac{\Gamma (\nu + \alpha + 1)}{\Gamma (\nu + 1) \Gamma (\alpha + 1)} f^\nu (\omega - \omega_0 - \nu \omega_c) \quad (9) \]

where \( \alpha = -2\delta B/\pi + (\delta B/\pi)^2 \), \( \Gamma(x) \) is the gamma function and \( f^\nu (x) \) is a distribution of width \( \varepsilon \) that tends to a delta function as \( \varepsilon \rightarrow 0 \).

The calculation of the emission spectrum proceeds in an analogous way. Initially the system is in the ground state \( |G\rangle \) of the full Hamiltonian \( H \) with a hole in the localized level. The transition rate is given by

\[ W_e (\omega) \propto \sum_j |\langle f | c_0 (0) | G \rangle|^2 \delta (\omega - \omega_0 - E_0' - E_f), \]

where \( E_0' \) is the ground state energy of \( H \), or

\[ W_e (\omega) \propto \text{Re} \int_0^\infty dt e^{-i\omega t} F_e (t), \quad (10) \]

where

\[ F_e (t) = e^{i\omega t} \langle G | e^{iH_1 t/\hbar} c_0^\dagger (0)e^{-iH_1 t/\hbar} c_0 (0) | G \rangle. \quad (11) \]

The initial Hamiltonian for emission is the final Hamiltonian for absorption and vice versa, i.e. \( H'_f = H_f, H'_i = H_i \). Furthermore the ground states of the Hamiltonians before \( |G\rangle \) and after the emission \( |G_0\rangle \) are related by \( |G_0\rangle = T |G\rangle \), where \( T \) is the unitary transformation \( F_e \). This allows us to arrive at

\[ F_e (t) = e^{i\omega t} \langle G_0 | a_0^\dagger (0, t)a_0 (0, 0) | G_0 \rangle, \]

where \( a_{m_\theta} (\theta, t) \) is again given by equation \( F_a \).

The rest of the calculation proceeds exactly as in the case of absorption and we find

\[ F_e (t) = e^{-i\omega t} F_a (t). \]

The emission spectrum \( W_e (\omega) \) has the same form as equation \( F_a \), with \( n\omega_c \) replaced by \( -n\omega_c \).
Thus, both the emission and absorption spectra consist of sets of peaks with intensities proportional to $\frac{\Gamma(n+\alpha+1)}{\Gamma(n+1)\Gamma(\alpha+1)}$. This is the central result of this paper. The emission spectrum is illustrated in Fig. I.

In the limit $B \to 0$ (that amounts to $\omega_c \to 0$ and $\nu \to \infty$), in a small $\omega$ interval there will be a number $n \gg 1$ of consecutive peaks. Then, by using the asymptotic formula $\frac{\Gamma(n+\alpha)}{\Gamma(n)} \sim n^\alpha$ for $n \gg 1$, we can see that the envelope of the emission peaks tends to the standard result $I(\omega) \sim \left(\frac{\omega}{\omega_c}\right)^\alpha$. Since physically $\varepsilon^{-1}$ must be of the order of the band width, which means $\varepsilon \sim \frac{1}{\nu} = \frac{B \hbar \rho S}{N \hbar \omega_c}$, the constant $\varepsilon/\omega_c \sim \hbar \rho F S/N$ plays the role of a field-independent, non-universal cutoff constant.

When $B \neq 0$ there is a single parameter $\alpha$ governing the relative intensities of the peaks similarly to the zero field case. What occurs here is that for $\alpha < 0$ there is an enhancement of the emission intensity due to the enhancement of the number of final states in this type of process. On the other hand, for $\alpha > 0$ we observe a reduction on the emission intensity that can be related to the Anderson orthogonality catastrophe. We emphasize, however, that the well-known power-law singularities of the $B = 0$ case are absent when the magnetic field is turned on. This can be traced back to the appearance of an energy gap, the cyclotron energy, $\hbar \omega_c$, which preempts the infrared divergence present when $B = 0$. Nevertheless, a remnant of this effect can still be seen in the envelope function of the discrete peaks in Fig. I. This is in agreement with the numerical results of Uenoyama and Sham in the case of infinite hole mass and with the experimental results of Skolnick et al.

In conclusion, we have used the bosonization technique for calculating exactly the emission and absorption spectra for transitions between a localized level and the discrete Landau levels of a two-dimensional electron gas. The intensities of the (equidistant) spectral lines follow an envelope function which is reminiscent of the singular behavior for zero magnetic field. A single parameter $\alpha$ determines the line intensities, and this parameter is nothing else than the exponent of the zero field edge singularity.

We would like to thank J. A. Brum for fruitful conversations. H.W. acknowledges full support from the Fundação de Amparo à Pesquisa do Estado de São Paulo (FAPESP). A.O.C. is grateful for partial support from the Conselho Nacional de Desenvolvimento Científico e Tecnológico (CNPq). D.B. wishes to thank FAPESP for support during his visit at UNICAMP, and M. Potemski for useful information about recent experimental results.

\begin{figure}[h]
\centering
\includegraphics[width=0.5\textwidth]{figure1.png}
\caption{Emission spectra for $\nu = 10$ and $\varepsilon = 0.1$ with $\omega$ measured from the threshold. The envelope of the peaks is reminiscent of the $B = 0$ case.}
\end{figure}

1. G. D. Mahan, Many-Particle Physics (Plenum Press, New York, 1981).
2. P. W. Anderson, Phys. Rev. Lett. 18, 1049 (1967).
3. G. D. Mahan, Phys. Rev. 153, 882 (1967); 163, 612 (1967).
4. P. Nozières and C. T. de Dominicis, Phys. Rev. 178, 1097 (1969).
5. K. D. Schotte and U. Schotte, Phys. Rev 182, 479 (1969).
6. S. Tomonaga, Prog. Theor. Phys. (Kyoto), 5, 544 (1950).
7. G. D. Mahan, in Solid-State Physics, edited by H. Ehrenreich, F. Seitz and D. Turnbull (Academic, New York), vol. 29, p. 75 (1974).
8. M. S. Skolnick et al., Phys. Rev. Lett. 58, 2130 (1987).
9. J. Gavoret et al., J. Phys. (Paris) 30, 987 (1969); E. Müller-Hartmann, T. V. Ramakrishnan and G. Toulouse, Phys. Rev. B 3, 1102 (1971).
10. T. Uenoyama and L. J. Sham, Phys. Rev. Lett. 65, 1048 (1990).
11. K. J. Nash et al., Phys. Rev. Lett. 70, 3115 (1993).
12. P. Hawrylak, Phys. Rev. B 42, 8986 (1990), B 44, 3821, 6262, 11236 (1991).
13. T. Uenoyama and L. J. Sham, Phys. Rev. B 39, 11044 (1989).
14. R. B. Laughlin, Phys. Rev. Lett. 50, 1395 (1983).
15. H. Westfahl Jr., A. H. Castro Neto and A. O. Caldeira, Phys. Rev. B 55, R7347 (1997), Z. Phys. B 103, 279 (1997).
16. J. M. Luttinger, J. Math. Phys. 4, 1154 (1963).
17. F. D. M. Haldane, J. Phys. C 14, 2585 (1981).
18. For a recent review see J. Voit, Rep. Prog. Phys. 58, 977 (1995).