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תכונות מסוימות של התגובה המגנטית
של מערכות מזוסקופיות קוונטיות

רומנס נארביץ'

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חיבור על מחקר

לשם מילוי חלקי של הדרישות לקבלת תואר
דוקטור למדעים

רומנס נארביץ'

הוגש לסנט הטכניון - מכון טכנולוגי לישראל

תמוז תשנ"ז חיפה יולי 1997

המחקר נעשה בהנחיית פרופ׳ אריק אקרמן בפקולטה לפיזיקה.

ברצוני להודות
לאריק אקרמן, על הנאה לעבוד איתו במשך שש שנים, על תשומת-הלב,
עידוד, ועזרה בדרכים רבות אחרות.
ליוסי אברון, על השיחות המרתקות ליד הלוח, על עזרתו.
לאוזי סמילנסקי, על הקיץ הנפלא במכון וייצמן למדע, על הבנתו.
לבוריס שפירא, על שיחות מועילות, על הספקנות.
לדומיניק ספנר, על שיתוף פעולה מעולה.
לשמואל פישמן, מיכאל מרינוב, רוברטו סולדטי, יאן פיודורוב, וילהלם
צברגר, על שיחות מועילות.
לאופיר אוסלנדר, הילה נחליאלי, סער רהב, דימיטרי גנגרדט, אלקסנדר
אלגרט, על עזרה בשלבים שונים של העבודה.
לנטע כהן, גדי טרליוק, יובל יאיש, יהודה רוט, ראובן פניני ,אוגני גורביץ׳,
שי שפירא, על נכונות לעזור ולדבר,
לאגלה על עזרה עם תיזה,
למשפחתי על תמיכתם.

תודתי לטכניון על העזרה הכספית הנדיבה.

תוכן עניינים

תקציר

עבודה זו מציגה מחקר על התגובה המגנטית של מערכות קוונטיות מזוסקופיות של גז אלקטרונים מנוונים כלוא בתחום מסוים של המרחב. התכונה החשובה ביותר של המערכת הקוונטית המזוסקופית היא קוהרנטיות קוונטית (quantum coherence) הנשמרת בכל התחום, כך שאורך הקוהרנטיות גדול מאורך אופייני של המערכת (בטמפרטורה מספיק נמוכה). לכאורה הקוהרנטיות המלאה מצביעה על צורך בספקטרום המדויק של המערכת כדי לחשב אפיוניה תרמודינמיים או קשורים להובלה. אך זה לא המקרה כאן ולכך שתי סיבות. הראשונה קשורה לאנרגיות אופייניות במערכות האלה. למרות שגודל של המערכת הוא סופי, המרחק בין רמות האנרגיה Δ הינו כל כך קטן, שכל טמפרטורה סופית (בתנאי מעבדה), בלי לערער את הקוהרנטיות, תהייה גדולה ביחס ל-Δ, ולכן הספקטרום ימרח. הסיבה השניה קשורה למגבלות הידע על הספקטרום המדויק. אכן, כתוצאה מזיהומים בתוך המערכת ומצורת השפה, לא ניתן לקבוע את הספקטרום המדויק, להוציא מקרים יוצאי דופן של המערכות האינטגרביליות. מסיבות אלה מודדים בדרך כלל את התכונות הספקטרליות הגלמיות. מטרת המחקר היא לפתח שיטות תאורטיות המתאימות לתיאור של התגובה המוחלקת (או המרוחה).

קיימות מספר שיטות לפתרון בעיה זו, העיקריות בהן, תורה של מטריצות אקראיות (RMT), פיתוחים הפרעתיים באי-סדר חלש (משטר דיפוזיוני), גישות לא-פרטורבטיביות המסתמכות על שימוש בתורות השדה כמו גישת סופרסימטריה, או קירובים סמי-קלאסיים המבוססים על נוסחת גוצוילר (Gutzwiller) של צפיפות המצבים. לכל

אחת מהשיטות האלה יש מיגבלות משלה. חלקן מזניחות תכונות ספקטרליות מיקרוסקופיות שעשויות להיות חשובות גם אחרי המריחה של הספקטרום (כמו RMT, או דיפוזיה), באחרות מתקבלת תשובה כל כך סבוכה שקשה להעריך אותה אלא בשיטות נומריות.

אנו מתמקדים בפיתוח גישה אחרת המבוססת על שיטות אסימפטוטיות לצורך תיאור התגובה המגנטית של המערכות האלה. זאת הנקודה המרכזית של המחקר. למרות שאנו מאמינים גישות אלה ישימות גם כאשר קיימת האינטרקציה בין האלקטרונים, אנו נתמקד בבעיה חד-חלקיקית. רק בפרק האחרון נדון בקצרה בפיסיקה של אפקט הול הקוונטי (Quantum Hall Effect). נושא חשוב אחר בעבודה הזאת הוא הסיבות לבחירה זו או אחרת של תנאי שפה במערכת מזוסקופית. אנו טוענים שבעית תנאי השפה הינה תאוריה אפקטיבית כאשר לא ניתן לפטור את השאלה ישירות בגלל קשיים מתמטיים או חוסר מידע פיסיקלי.

אחד הכלים היעילים לחקר תופעות של קוהרנטיות קוונטית הינו שדה מגנטי, מכיוון שהוא משפיע על פזות של פונקציות גל אלקטרוניות. כתוצאה מכך, לגדלים תרמודינמיים שונים יש תלות מעניינת בשדה המגנטי. מלבד המקרה של שדה אחיד, נדון גם בפוטנציאל ווקטורי של הסליל האידיאלי, שאלקטרונים אינם יכולים לחדור לתוכו, הנקרא שדה של אהרונוב-בוהם (Aharonov-Bohm).

להלן נציג את התוכן של הפרקים. שני הפרקים הראשונים מוקדשים לחקר התגובה המגנטית לשדה אהרונוב-בוהם. אנו מתחילים בדיון על זרמים מתמידים (או מגנוט), הזורמים בטבעות נקיות או לא מסודרות. מקורם של הזרמים האלה בקוהרנטיות הקוונטית, לכן הם נמדדים בטמפרטורות קטנות , כך שמרחק

הקוהרנטיות יהיה גדול יותר מההיקף של הטבעת. בטמפרטורות כאלה (שהן מסדר גודל של קלוין) יש חשיבות לסטטיסטיקה של החלקיקים. אנו עובדים בצבר גרנד-קנוני ולכן משתמשים בהתפלגות של פרמי-דירק (Fermi-Dirac). הזרם המתמיד שהוא נגזרת של פוטנציאל טרמודינמי לפי השטף המגנטי, נתון על ידי פונקציה של השטף ושל פוטנציאל כימי עם אוסצילציות חזקות (לא מונוטונית).

אנו מפתחים את הפונקציה בשטף המגנטי, כאשר כל סדר בפיתוח הזה תלוי בפוטנציאל כימי בלבד. הטענה העיקרית היא שניתן להציג כל סדר בתור סכום של שני חלקים. חלק אחד תלוי בצורה מונוטונית ב-μ, חלק שני הוא פונקציה אוסצילטורית עם ממוצע אפס. החלוקה הזאת מקובלת בתורה סמי-קלאסית כאשר מדובר בצפיפות מצבים. כאן אנו משתמשים בה עבור גדלים אחרים, כאשר הדגש בעבודה הזו על החלק המוחלף (מונוטוני). אחת התוצאות החשובות היא שבניגוד לציפייה שהחלק הזה משקף תכונות מקרוסקופיות של המערכת, הוא נמצא רגיש גם לתופעות עדינות של התאבכות קוונטית.

אנו מראים שהזרם המוחלק בטבעות נקיות מתאפס. לאחר מכן אנו חוזרים על החישובים הקיימים של הזרם הממוצע בטבעות לא מסודרות. החישובים האלה לא מחדשים דבר מבחינתנו, כי עיקרם הוא מריחה של הזרם על ספקטרום של מערכת נקיה. אך ברור מאליו שלספקטרום של טבעת עם זיהומים תכונות שונות מהספקטרום של הטבעת הנקיה. לכן הזרם, שהוא גודל ספקטרלי, לא יכול להישאר בלתי תלוי בתכונות האלה (כמו ניוון והופעת פערים). על מנת להוכיח זאת, אנו מחשבים זרמים מוחלקים בשני מודלים חד-מימדיים, קרוניג-פני (Kronig-Penney) וסקרף (Scarf). לכל אחד מהמודלים האלה התנהגות ספקטרלית מיוחדת, שונה מזו של הטבעת הנקיה.

ואכן, רואים שהזרם לא מתאפס במקרה של מודל קרוניג-פני, וזה מחזק את טענתנו על חשיבות התכונות העדינות של הספקטרום לתגובה המגנטית הממוצעת. עם זאת, השאלה, איזה מאפיינים של הספקטרום גורמים לזרם להתאפס, נשארת פתוחה ודורשת חקירה נוספת.

מלבד המקרים החד-מימדיים, בהם המודלים הכוללים את הזיהומים הינם עדיין פשוטים מספיק לחישובים אנליטיים, איננו מכירים מודלים כאלה בשלושה מימדים. לכן אין לנו תוצאות מגובשות במקרים האלה. בשלושה מימדים קיימת תאוריה RMT לתיאור הספקטרום של המערכת הלא מסודרת. אולם, התיאוריה RMT נותנת את הספקטרום בטווח סופי של האנרגיה בלבד, בעוד שלטענתנו התכונות האסימפטוטית של הספקטרום הם שקובעות את הזרם המוחלק.

לצורך דיון על זרמים בטבעות אנו מניחים שפוטנציאל ווקטורי אינו תלוי במרחק בין החלקיק לסליל. חשוב להבין האם ההנחה הזו נשארת בתוקף כאשר מגדילים את עובי הטבעת. לצורך מטרה זו אנו חוקרים את התגובה המגנטית לשדה של הסליל האידיאלי במערכת פתוחה - מישור אין-סופי, כאשר הפוטנציאל הווקטורי נמצא ביחס הפוך עם המרחק בין החלקיק לסליל. התוצאות של חישוב הזרם המוחלק מצביעות על הבדל משמעותי בין מקרה זה לבין המקרה של טבעת צרה. הזרם המוחלק נשאר סופי ואינו מתאפס. קיים הבדל נוסף הקשור למגנוט. חשוב לציין, בעוד שבמישור האין-סופי הקשר בין המגנוט לזרם אינו פשוט, ויש לחשב את המגנוט בנפרד, במקרה של הטבעת המגנוט פרופורציוני לזרם.

הפרק הרביעי מוקדש לתיאור בעיית המיקום הקוונטי על ידי מודל של מהלך אקראי (random walk). אנו מוכיחים שמודל זה שנוסח על ידי אלן (Allen) אקוויוולנטי בגבול אסימפטוטי לגישה הדיאגרמטית של פולהרדט וולפלה (Vollhardt and Woelfle) לבעיית המיקום. לכן, מודל של מהלך אקראי נותן אותן תוצאות עבור אקספוננט קריטי של מרחק המיקום (localization length). מצד שני, התיאור של אלן מתאים למערכת מזוסקופית, עם או בלי שדה מגנטי, מכיוון שהגבול האסימפטוטי של מהלך אקראי שקול למשוואת דיפוזיה. לאחר מכן, אנו עוסקים בתגובה המגנטית של מערכות סופיות לשדה מגנטי אחיד (של ביליארדים מגנטיים).

בפרקים חמישי ושישי אנו מחשבים תכונות ספקטרליות של ביליארדים מגנטיים דו-מימדיים, שקשורות למצבי שפה ופנים המיוחדים למערכות האלה. בתיאור של מכניקה קלאסית אלקטרון נע בשדה מגנטי במסלול מעגלי. כאשר מסלול האלקטרון נמצא כולו בתוך הביליארד, אנו מדברים על מצב פנים, אם החלקיק פוגע בשפה, הוא מתחיל לנוע לאורכה כאשר הוא ממשיך להסתובב בקשתות קטנות. מסלול כזה נקרא מצב שפה. ההפרדה החדה בין מצבי גוש ושפה נעלמת בגבול הקוונטי. אנו חוקרים את ההיבט הזה במקרה של ביליארדים אינטגרביליים, בעזרת שיטות סמי-קלאסיות. על ידי התאמה אסימפטוטית של פונקציות גל סמי-קלאסיות, אנו מראים איך מצבי שפה מתחברים בספקטרום למצבי פנים. אנו מוצאים שהשיטות האלה מתארות בדיוק גבוה את רמות האנרגיה הכי נמוכות.

בפרק שישי אנו חוזרים לחלק המוחלק של התגובה המגנטית-מסלולית בביליארדים מגנטיים. מצבי שפה משפיעים גם על הגודל

הזה וגורמים לתיקון של הדיאמגנטיזם של לנדאו (Landau). התיקון הזה נמצא פרופורציוני לאורך השפה. אנו מחשבים אותו בשתי שיטות אסימפטוטיות שונות אשר נותנות אותה תוצאה. אנו מתקנים טעות בחישובו של רובניק (Robnik), שהשתמש באחת מהשיטות האלה.

בפרק השביעי אנו חוזרים על החישוב של דיאמגנטיזם של לנדאו במישור אין-סופי. הדוגמה הזו משמשת ככלי לחקירת קשר שקיים בין מריחה של הגודל הפיזיקלי על הספקטרום לבין קירוב שלו בעזרת שיטה של הריבועים המינימליים (least squares). אחר כך אנו מחשבים את התגובה לשדה מגנטי אחיד, כאשר גז אלקטרוני נמצא על כדור ועל מישור היפרבולי, ומוצאים אותה זהה לדיאמגנטיזם של לנדאו במישור. התגובה המסלולית אינה תלויה בעקמומיות קבועה של המשטח המשמש כתווך לחלקיקים.

בפרק האחרון נשאלת השאלה: "איך בוחרים תנאי שפה לבעיה פיזיקלית?" לדעתנו לשאלה הזו לא מייחסים חשיבות מספקת, ולא תמיד יש לבחירה מסוימת של תנאי שפה מוטיבציה פיזיקלית. אנו נראה שבמיקרים מסוימים, שבהם חסר מידע מלא על המערכת, ניתן לבחור , מתוך שיקולים פיזיקליים, תנאי שפה שמפשטים את הבעיה ובכך מאפשרים לפתור אותה. אחרי השיקולים הכלליים האלה אנו דנים באפקט הול קוונטי (שדה מגנטי חזק מאוד בביליארד מגנטי) ומציעים תנאי שפה לא מקומיים, שבעזרתם אפשר להקנות למושגים של מצבי שפה וגוש משמעות מדויקת. למצבים האלה, כפי שהוגדרו על ידי תנאי שפה שבחרנו, יש את תכונות הפיזיקליות הנדרשות: מצבי פנים מנוונים וערעורים של מצבי שפה ללא פער אנרגטי. אנו דנים בשתי בחירות של תנאי שפה: אטיה-פטודי-זינגר (Atiyah-Patodi-Singer) ותנאי שפה קירליים. הבחירה הראשונה מכילה תכונות

מתמטיות יפות, הקשורות במשפטי אינדקס (index theorems), אך הספקטרום שלה אינו פונקציה רציפה של פרמטרים חיצוניים (לדוגמה, שטף של אהרונוב-בוהם). לכן אנו מציעים וחוקרים תנאי שפה קירליים עם ספקטרום רציף ששומר על דואליות קוונטית בין שפה לפנים.

SOME PROPERTIES OF THE MAGNETIC RESPONSE OF MESOSCOPIC QUANTUM SYSTEMS

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SOME PROPERTIES OF THE MAGNETIC RESPONSE OF MESOSCOPIC QUANTUM SYSTEMS

RESEARCH THESIS

SUBMITTED IN PARTIAL FULFILLMENT OF THE REQUIREMENTS
FOR THE DEGREE OF DOCTOR OF SCIENCE
IN PHYSICS

BY

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SUBMITTED TO THE SENATE OF THE TECHNION - ISRAEL INSTITUTE OF TECHNOLOGY
TAMUZ 5757 HAIFA JULY 1997

This research was carried out in the Physics department of the Technion under the supervision of Prof. Eric Akkermans.

I wish to thank Eric Akkermans for the pleasure to work with him for these six years, for his caring, encouraging, helping in many other ways,
Yosi Avron, for memorizable moments working in his company, for his help,
Uzy Smilanski, for the wonderful summer at Weizmann Institute of Science, for his courtesy,
Boris Shapiro, for useful discussions, for his scepticism,
Dominique Spehner, wonderful collaborator,
Shmuel Fishman, Michael Marinov, Roberto Soldati, Yan Fyodorov, Wilhelm Zwerger for useful discussions,
Hila Nahlieli, Ophir Auslaender, Saar Rahav, Dimitry Gangardt, Alexander Elgart, for the help at various stages of the work,
Yehuda Roth, Reuven Pnini, Evgeni Gurevich, Neta Cohen, Nir Gov, Gadi Terliuk, Yuval Yaish, Shye Shapira for being ready to help or to chat,
Egle, for the help with the thesis,
my family, for helping me to keep going.

The generous financial support of the Technion is gratefully acknowledged.

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Abstract

Various problems dealing with the magnetic response of mesoscopic quantum systems of degenerate electrons confined in a domain are considered. A mesoscopic quantum system is a system which keeps its full quantum coherence over the whole domain. It is argued that important characteristics of such a system does not presuppose the knowledge of the exact energy spectrum for two reasons. Although the system is finite and has therefore a discrete spectrum, the level spacing is so small that any finite temperature in a realistic range although keeping the quantum phase coherence, will always smooth the spectrum, so that the individual levels will not be resolvable. The second reason is connected with our limited knowledge of the exact spectrum. Indeed, due to inherent bulk disorder, to the shape of the boundaries among other factors, the exact spectrum is not known in principle except perhaps in a limited number of so called integrable systems. For those reasons, only gross features of those spectra are measured. Asymptotic methods are developed in this thesis in order to describe this smoothed response due either to a uniform magnetic field or, an Aharonov-Bohm vector potential.

We consider the problem of persistent current (magnetization) flowing in clean or disordered rings. We observe that the disorder average of the persistent current is equivalent to smoothing of the current over the spectrum of a clean ring. This leads us to consider the smooth current in models with impurities, like the Kronig-Penney model. The results show that the smooth quantities are sensitive to such properties of the spectra as gaps and degeneracies. They are also sensitive to an approximation of the genuine Aharonov-Bohm field by a global gauge transformation, as a calculation in an open system shows.

The random walk description of quantum localization as an asymptotic method is presented. The self-consistent diagrammatic approach to calculate the critical exponent of the localization length is shown to be equivalent to the random walk picture, proposed by Allen. The critical exponent is obtained by an asymptotic properties of the random walk. Since the asymptotic limit of random walk is the diffusion equation, we formulated the quantum localization as a boundary value problem.

Then, we study the magnetic response of bounded systems in a uniform magnetic field (magnetic billiards). The spectral properties of such magnetic billiards reflecting the interplay between the magnetic field and the boundary of these domains are calculated. The necessity to distinguish between smooth contribution and oscillations is emphasized. In particular the smooth part of the density of states for the semi-infinite cylinder is found by two different methods. On the other hand the classical picture of the edge and bulk states in the strong magnetic field is examined from the point of view of quantum mechanics. To this aim we use semi-classical

methods to calculate the energies of the lowest Landau level in two separable billiards - semi-infinite plane and disc. The method of asymptotic matching of the WKB wavefunctions and the comparison equation method are applied respectively, working surprisingly well even for the lowest energies.

The smooth part of the spectrum yielding the Landau diamagnetic susceptibility is a paradigm to deepen our understanding of the notion of smoothing over the energy of some thermodynamic quantity. The connection between smoothing and approximating the exact quantity by the least squares procedure is raised. It is shown that the smooth diamagnetic response of the electron gas on the sphere and on the hyperbolic plane are identical to those of the plane, being therefore independent of the curvature of the surface.

Finally, the question "how to choose boundary conditions?" is raised. We develop the point of view that the boundary conditions should serve as an effective theory in problems that are either too difficult to solve as they stand, or with insufficient information about the system. In particular in the Quantum Hall regime boundary conditions are desirable, which reflect edge-bulk duality inherent in this problem. This requirement is shown to be satisfied by non-local boundary conditions. Two choices of non-local boundary conditions are studied, the so-called Atiyah-Patodi-Singer and the chiral boundary conditions. The former choice guarantees the existence of Index theorems, which we use to propose a new relation for the Hall conductance. However there the energies are not continuous functions of external parameters (like an Aharonov-Bohm flux), thus obstructing the discussion of adiabatic transport. On the other hand, the chiral boundary conditions give a continuous spectrum, which preserves the bulk-edge separation, and provide appealing physical properties to bulk and edge.

List of Symbols

symbol	meaning
$\mathbf{A}$	vector potential;
Ai	Airy function of the first kind;
Bi	Airy function of the second kind;
β	inverse temperature;
c	annihilation operator;
$c^\dagger$	creation operator;
d	dimension;
$D(\mathbf{q},\omega)$	diffusion coefficient;
D	annihilation operator in the Landau level;
$D^\dagger$	creation operator in the Landau level;
D_ν	parabolic cylinder function;
Δ	energy level spacing;
E	energy;
e	reduced energy;
$f(E)$	Fermi-Dirac distribution;
${}_1F_1$	confluent hypergeometric function;
Φ	magnetic flux;
φ	reduced magnetic flux;
g	monopole charge;
$g(s)$	regularized resolvent;
$G(E)$	Green's function;
Γ	gamma function;
H	Hamiltonian;
I	current;
i	reduced current;
$\mathbf{j}$	current density;
J_p	Bessel function;
k	wavevector;
l	angular momentum quantum number;
m	mass of the electron;
M	magnetic moment;

symbol	meaning
μ	chemical potential;
n	particle density;
N	number of particles;
p	momentum;
$P(t)$	heat kernel;
ψ	wavefunction;
Ψ	digamma function;
$\mathcal{Q}$	grand-canonical partition function;
R	radius of a ring;
r_c	cyclotron radius;
$\rho(E)$	density of states;
$S(n)$	probability to visit n distinct sites;
σ	conductance;
σ_H	Hall conductance;
T	temperature;
τ	transport elastic scattering time;
v	velocity;
V	potential;
W	hopping;
Ω	thermodynamic potential;
ω	cyclotron frequency;
$\chi(\mathbf{q},\omega)$	density-density response function;
χ	magnetic susceptibility;
ζ	zeta function.

Chapter 1

Introduction.

We consider in this thesis various problems dealing with the magnetic response of mesoscopic quantum systems of degenerate electrons confined in a domain. By mesoscopic quantum system, we mean a system which keeps its full quantum coherence all over the domain, i.e. such that the so-called phase coherence length is larger than the size of the system (at low enough temperature). The fact that the system keeps its full quantum coherence seems to indicate that in order to calculate its characteristics, either thermodynamical or transport properties, we need to know the exact energy spectrum, like for instance in related problems in atomic physics. It is not the case here and for two reasons. The first one is related to the characteristic energy scales of those systems. Although the system is finite and has therefore a discrete spectrum, the level spacing Δ is so small that any finite temperature in a realistic range although keeping the quantum phase coherence, will always be larger than Δ and therefore will smooth the spectrum. The second reason is connected with our limited knowledge of the exact spectrum. Indeed, due to inherent bulk disorder, to the shape of the boundaries among other factors, we do not know in principle the exact spectrum except perhaps in a limited number of so called integrable systems. For those reasons, we measure usually only gross features of those spectra. And the theoretical challenge is to develop methods in order to describe this smoothed response. This is precisely the aim of this thesis.

Well known and successful methods have already been applied to this problem. We may mention, among others the Random Matrix theory, perturbation expansion for weak disorder (the so-called diffusive regime), non-perturbative field-theoretic approaches like supersymmetry, or semi-classical expansions essentially based on the Gutzwiller formula for the density of states. Each of those methods has its limitations. Some of them do ignore microscopic features of the spectrum which might still be relevant after smoothing (like RMT, or diffusion), or that it may loose important spectral information by artificially truncating infinite series, or more prosaically that some may give precise answer but are difficult to evaluate other than numerically.

Here we focus our attention on the development of another point of view based on asymptotic methods to the study of the magnetic thermodynamic response of those systems. This is the guideline of all this work. Although we believe that it

has a larger field of application, we shall mostly restrict ourselves to the case of non-interacting systems (including Fermi liquids). Only in the last chapter, we shall make a brief incursion in the physics of Fractional Quantum Hall effect.

Another theme of this thesis is the motives of choosing one or another boundary condition in an idealized problem of quantum-mechanical motion in the mesoscopic regime. In particular we suggest to widen the usual physicist's choice of boundary conditions in allowing for non-local ones, which are shown to be legitimate from the mathematical point of view and could also be physically motivated.

An efficient tool to investigate quantum coherence effects in electronic systems is the phase sensitivity of the electronic wave functions to the magnetic field. The magnetic response of isolated finite-size systems is the main subject of research in this work. The electron gas can be acted upon by a uniform magnetic field or, conversely, by the vector potential due to an ideal magnetic coil, which is impenetrable for the electrons (an Aharonov-Bohm field). The main effect of the magnetic vector potential is to break the time-reversal invariance causing thus a phase difference in time-reversed quantum amplitudes. Because of quantum coherence, this gives rise to magnetic field dependence of physical quantities. In the following we present the outline of the thesis.

The next two chapters are devoted to the study of the magnetic response in a setup peculiar to the Aharonov-Bohm effect. We start our discussion by formulating the problem of finding the persistent current (or the magnetization) flowing in clean or disordered rings. To observe these thermodynamic currents, originating from the phase coherence of the electronic wave function, the temperature should be sufficiently low to keep the coherence length of the order of the circumference of the ring. At these sub-Kelvin temperatures the statistics of the particles becomes important. We work within the grand-canonical ensemble, and therefore use the Fermi-Dirac distribution.

Considering the persistent current, which is the magnetic flux derivative of the grand-canonical potential, we immediately encounter the following problem - the current fluctuates both as a function of flux and chemical potential. We expand this function for small flux, and argue that as a function of the chemical potential, the persistent current possesses two parts, a smooth one and oscillations (this point of view seems to be accepted in quantum chaology, when the density of states is considered). This remark, no matter how trivial it may seem is in our opinion very important. It seems that several authors are not sufficiently aware of which part of a thermodynamic quantity they are dealing with. We limit ourselves to the smooth magnetic response. The smooth quantities are generally supposed to reflect only macroscopic properties of a system, therefore it is important to notice that they are also sensitive to the subtle effects of quantum coherence.

First the clean ring is considered, then we critically review the existing calculations of the current in disordered rings. It is surprising to find that all known to us works on disordered rings do nothing else but smoothing out the clean system current. However it is clear that the spectrum of the disordered ring is very different from that of a clean system. Therefore we calculate the smooth persistent currents in two models of one-dimensional systems, Kronig-Penney and Scarf, possessing cer-

tain features of their spectra that distinguishes them from the clean one-dimensional ring (like gaps opening instead of degeneracies of a clean system). Indeed we find that the current is sensitive to those properties of the spectrum. It is much more difficult to deal with three-dimensional rings, because their spectrum is not available. We show that problems arise when the weak disorder perturbation theory is applied to calculate the persistent current. Since the statistical properties of the disordered system spectrum is well described in terms of Random Matrix theory, it should be of some help to this problem. We also discuss the smooth magnetic response in the canonical ensemble as opposed to the grand-canonical calculation.

The vector potential of an ideal coil (Aharonov-Bohm flux line) is assumed to be coordinate independent in the above calculations (it is equivalent to a global gauge transformation). It is however important to understand how realistic is this approximation if the ring has many transverse channels. Having this in mind, we consider in the third chapter the magnetic response to an ideal coil piercing the infinite plane, the vector potential being inversely proportional to the distance from the coil. It should be noted that in this case the magnetization is not simply related to the current and should be calculated separately. The results show marked difference from those in the coordinate independent vector potential case. Whereas the smooth current in a clean system was zero, for the infinite plane we find non-zero currents. Furthermore our calculation clearly shows the asymptotic character of the persistent current, a point which was not clear before.

The fourth chapter is devoted to the random walk description of quantum localization. First we review the self-consistent diagrammatic approach to calculate the critical exponent of the localization length. It is shown to be equivalent to the localization criterion formulated by Allen, based on the random walk picture, from which the critical exponent follows using the asymptotic properties of the random walk. The asymptotic limit of random walk being the diffusion equation, we again make contact with the main theme of the thesis, formulating the quantum localization as a boundary value problem. The connection to the large n limit of the n-component classical Heisenberg model with $O(n)$ symmetry is mentioned.

Then, we study the magnetic response of bounded systems in a uniform magnetic field (magnetic billiards). In chapters 5 and 6 we calculate the spectral properties of such magnetic billiards due to the interplay between the magnetic field and the boundary of these domains. On one hand we stress again the necessity to distinguish between smooth contribution and oscillations. On the other hand the classical picture of the edge and bulk states in the strong magnetic field is examined from the point of view of quantum mechanics. To this end we use semi-classical methods to calculate the energies of the lowest Landau level in two separable billiards - semi-infinite plane and disc. The method of asymptotic matching of the WKB wavefunctions and the comparison equation method are applied respectively, working surprisingly well even for the lowest energies.

In the sixth chapter we calculate the smooth part of the density of states for the semi-infinite cylinder. We propose two different methods to perform the calculation, both giving the same result. Our main interest is in the term proportional to the length of the boundary which has in addition a magnetic field dependence. This

term gives a perimeter correction to the Landau diamagnetism, an expression which corrects a result obtained by Robnik.

The smooth part of the spectrum yielding the Landau diamagnetic susceptibility is studied in chapter 7, where we try to deepen our understanding of the notion of smoothing over the energy of some thermodynamic quantity. Taking as an example the thermodynamic potential, we show that the calculation of a smoothed quantity is equivalent to approximating the exact quantity by the least squares procedure. In the sequel of this chapter we show that the smooth diamagnetic response of the electron gas on the sphere and on the hyperbolic plane are identical to those of the plane, being therefore independent of the curvature of the surface.

In the last chapter we try to answer the question "how to choose boundary conditions?". We feel that not enough thought is devoted to the question of physical motivation for a particular choice of boundary conditions. We develop the point of view that the boundary conditions should serve as an effective theory in problems that are either too difficult to solve as they stand, or with insufficient information about the system. After some general arguments, we turn to the Quantum Hall regime (strong magnetic field) and argue that if one is willing to use non-local boundary conditions, the possibility arises to define precisely the edge and the bulk of a Quantum Hall system. Those definitions should shed some light on the edge versus bulk controversy of the theory of the Quantum Hall effects. Two choices of non-local boundary conditions are studied, the so-called Atiyah-Patodi-Singer and the chiral boundary conditions. The former choice guarantees the existence of Index theorems, which we use to propose a new relation for the Hall conductance. However there the energies are not continuous functions of an external parameter (like an Aharonov-Bohm flux), thus obstructing the discussion of adiabatic transport. On the other hand, the chiral boundary conditions give a continuous spectrum, which preserves the bulk-edge separation, and provide appealing physical properties to bulk and edge.

Chapter 2

The average persistent current in a small metallic ring.

2.1 Generalities.

To define the problem, consider a small weakly disordered metallic ring (the properly defined phase coherence length should exceed the circumference of the ring $2\pi R$, where R is the radius) placed in a weak magnetic field and we measure its magnetic response. In the limit of a thin ring, of width w much less than R, electrons can be assumed to move in a field free medium, all magnetic field contained in the hole (Figure 2.1). This approximation seems quite natural in the semi-classical picture, which should hold for electrons moving with Fermi velocity v_F. The information necessary to calculate the semi-classical thermodynamic quantities is related to classical periodic orbits, more precisely, their stability properties and the actions associated with them are needed. The only modification in the presence of a weak magnetic field is the additional term in the action equal to the magnetic flux, encircled by the periodic orbit [1]. In a thin ring, there are two classes of orbits - those that wind around the hole and those that do not. The first class subtends the area, proportional approximately to an integer times the cross-section of the hole, the area subtended by the second class loops is smaller and negligible. Since the magnetic flux is proportional to the area encircled, this justifies our approximation.

Hence the setup characteristic of the Aharonov-Bohm (A-B) effect [2] is electrons moving in a field-free domain, subjected to the vector potential of a thin coil threading the ring, the magnetic field contained perfectly inside the coil. This vector potential is an azimuthal field taken usually equal to

$$A_\theta = \frac{\Phi}{2\pi r}, \tag{2.1}$$

where Φ is the magnetic flux in the coil. The one-electron Schrödinger equation to be solved is most conveniently written down in the cylindrical coordinates

$$-\frac{\hbar^2}{2m}\left(\frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial}{\partial r}\psi\right)+\frac{1}{r^2}\left(\frac{\partial}{\partial\theta}-i\varphi\right)^2\psi+\frac{\partial^2}{\partial z^2}\psi\right)+V(\mathbf{r})\psi=E\psi, \tag{2.2}$$

here $V(\mathbf{r})$ is the random potential, $\varphi = \Phi/\Phi_0$ is the magnetic flux, measured in units of elementary flux quantum $\Phi_0 = hc/e$. The following assumptions are made about the disorder potential: it has a vanishing average $\langle V(\mathbf{r})\rangle = 0$, it is δ-correlated $\langle V(\mathbf{r})V(\mathbf{r}')\rangle = \gamma\delta(\mathbf{r}-\mathbf{r}')$, with $\gamma = 1/2\pi\tau\rho(\mu)$, here τ is the transport elastic scattering time, $\rho(\mu)$ is the density of states at the Fermi energy. It is important to note that the gauge transformation $A_\theta \to A_\theta - \Phi/2\pi r$ (which for the wave-function means $\psi \to e^{-i\varphi\theta}\psi$) reduces (2.2) to the magnetic flux independent equation. However as it should be, Φ does not disappear from the problem, modifying periodic boundary condition in the following way

$$\psi(r,\theta+2\pi) = e^{i2\pi\varphi}\psi(r,\theta). \tag{2.3}$$

The electrons motion in the ring due to the magnetic field gives a finite magnetization. In the limit of a very thin ring, this magnetization equals the current flowing along the circumference times the area subtended by the ring. This current is purely thermodynamic, non-dissipative, and usually named "persistent current" [3]. The current density in the n'th quantum state is from the continuity equation

$$j_\theta = \frac{\hbar}{m}\mathrm{Im}(\psi_n^*\frac{1}{r}\frac{\partial}{\partial\theta}\psi_n - i\frac{\varphi}{r}\psi_n^*\psi_n). \tag{2.4}$$

On the other hand, using perturbation expansion in the reduced flux φ, we obtain from the first order term of the energy:

$$\frac{dE_n}{d\varphi} = i\frac{\hbar^2}{m}\int d\theta\frac{dr}{r}\psi_n^*(\frac{\partial}{\partial\theta} - i\varphi)\psi_n. \tag{2.5}$$

The current is by symmetry the radial integral of the current density $I_n = \int dr j_\theta$. Substituting (2.4) in this equation and comparing with (2.5), we get the following formula for the persistent current flowing in the n'th state

$$I_n = -\frac{c}{e}\frac{\partial E_n}{\partial\Phi}. \tag{2.6}$$

Due to the presence of $V(\mathbf{r})$ equation (2.2) still poses a difficult problem (with the exception of the clean ring to be treated later), therefore an additional approximation is made. The ring is cut and straightened up to a rod. The rod is then copied an infinite number of times along the x direction to give a lattice with the initial rod as the unit cell. An electron in the lattice moves according to the usual Schrödinger equation with the periodic potential $V(x,y,z) = V(x+2\pi R,y,z)$. Within the unit cell this potential is random with previously stated properties. Bloch theorem [4] holds for this periodic Hamiltonian, so that to each eigenstate ψ a wave vector k is associated $\psi(x+2\pi R,y,z) = e^{i2\pi Rk}\psi(x,y,z)$. Using $\psi \to e^{ikx}\psi$, the Schrödinger equation acquires the form

$$-\frac{\hbar^2}{2m}((\frac{\partial}{\partial x} - i\hbar k)^2 + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2})\psi + V(\mathbf{r})\psi = E\psi. \tag{2.7}$$

The wave vector k is therefore parallel to the reduced magnetic flux φ. The analogy goes as far as the connection of the current with the derivative of the energy. As is

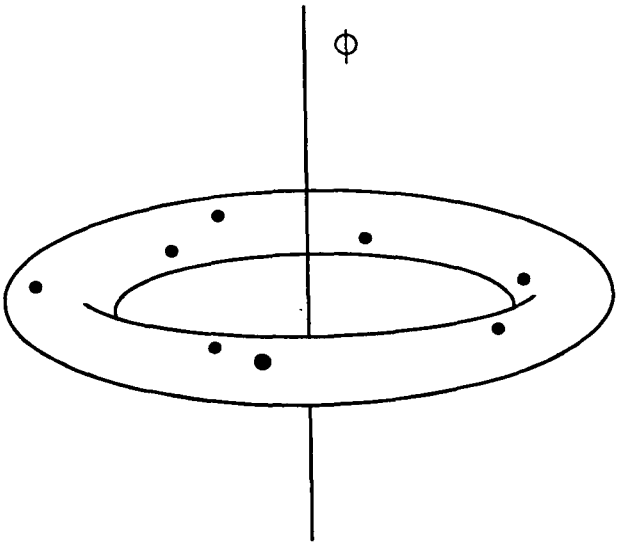

Figure 2.1: Schematic drawing of the problem setup.

well known, the mean velocity of the Bloch electrons is given by $v_n = \partial E_n/\partial(\hbar k)$, a relation equivalent to (2.6). Equation (2.7) is what we will consider from now on, using the notation φ/R for $\hbar k$ (mention has to be made that equations (2.2) and (2.7) are equivalent in the case of one spatial dimension).

Finally we would like to list three general properties, common to both A-B and Bloch problems. These are known as Byers-Yang theorems [5].

1. The energy levels are periodic functions of φ with period 1 (this follows from the formulation, where the flux enters only through the boundary conditions (2.3)).

2. The energy levels are even functions of φ (this follows when taking the complex conjugate of the Schrödinger equation).

3. The partition function is an even periodic function of φ with period 1.

2.2 The clean one-dimensional ring.

A very useful exercise to do before getting to more complicated calculations in the disordered ring is to consider a one-dimensional clean ring, threaded by the flux carrying coil. In this simple system the persistent currents can easily be found explicitly [6]. The one-electron Schrödinger equation is just (2.2) or (2.7) adapted for one-dimension. The conserved angular momentum will be denoted by l. The energies of the eigenstates are

$$E_l = \frac{\hbar^2}{2mR^2}(l-\varphi)^2. \tag{2.8}$$

The persistent current in this eigenstate is according to (2.6)

$$I_l = \frac{\hbar}{2\pi m R^2}(l - \varphi). \tag{2.9}$$

The total current I is equal to the sum of I_l over occupied eigenstates. Suppose for simplicity that the temperature is zero and there are N electrons in the ring. Ignoring the spin, we have to populate the N lowest energy eigenstates as required by the Fermi principle. Because of Byers-Yang theorems the persistent current is a periodic odd function of φ with the period 1. If the number of electrons N is odd, the total current is

$$I = -\frac{N\hbar\varphi}{2\pi m R^2} \qquad -0.5 \leq \varphi < 0.5, \tag{2.10}$$

therefore it is a discontinuous function at the half-integer values of φ. We call this current diamagnetic, because it is negative when the reduced flux is a small positive number. If on the other hand N is even, the current turns out to be

$$I = -N\hbar(\varphi - 1/2)/2\pi m R^2 \quad 0 \leq \varphi < 1. \tag{2.11}$$

The discontinuities in this case occur at the integer φ's. This current is paramagnetic, being positive for small positive reduced flux. Instead of keeping the number of particles fixed, we could attach the ring to a reservoir of electrons, thus imposing a constant chemical potential μ in the ring. Then, as φ is varied, the number of electrons can change - an electron can escape to the reservoir or alternatively it can flow from the reservoir into the ring. This happens, when the energy of the electronic eigenstate coincides with the chemical potential μ at some value φ^* of flux. Because of Byers-Yang theorems, for the flux $1 - \varphi^*$, the number of electrons changes again, so that at $\varphi = 2\pi$ it is identical to $N(\varphi = 0)$ (in the one-dimensional ring N can change discontinuously only twice in the interval $0 \leq \varphi < 2\pi$). The persistent current will have discontinuities at $\varphi = \varphi^*$ and $\varphi = 1 - \varphi^*$, otherwise being similar to the constant N cases. This discontinuous nature of the total current in the grand canonical ensemble (constant μ) is quite general, requiring only a discrete spectrum, and therefore also true for the disordered rings. It is of certain interest to calculate the average of the persistent current over the chemical potential, hence over the energy, because this could give some indication about the average over the disorder in the dirty rings. We should do the calculation for a non-zero temperature T in order to smooth out the singularities of the total current as a function of φ.

For the finite T case, the correct formula for the total grand canonical persistent current is

$$I = \sum_{l=-\infty}^{\infty} I_l f(E_l), \qquad f(x) = \frac{1}{e^{\beta(x-\mu)} + 1}, \tag{2.12}$$

with E_l and I_l given by (2.8) and (2.9) respectively, $f(x)$ - the Fermi-Dirac distribution. The current for the one-dimensional ring has been calculated before in the form of Fourier series [6], but we would like here to present another line of argument, which in our opinion can be generalized easier for more complicated cases.

Our argument is based on the use of the Euler-Maclaurin summation formula to sum (2.14). It is important to realize that when used to evaluate an oscillating

quantity, the Euler-Maclaurin formula smoothes out the oscillations, therefore when applied to calculate the persistent current, it should directly yield an average over the chemical potential. A reminder seems to be in place for the Euler-Maclaurin summation formula, which is to be understood in the asymptotic sense [7]

$$\sum_{k=1}^{n-1} F(k) \sim \int_0^n F(k)\,dk - \frac{1}{2}\{F(0)+F(n)\} + \frac{1}{12}\{F'(n)-F'(0)\} \qquad (2.13)$$
$$-\frac{1}{720}\{F'''(n)-F'''(0)\} + \cdots (-1)^{p-1}\frac{B_p}{(2p)!}\left\{F^{(2p-1)}(n)-F^{(2p-1)}(0)\right\} + \cdots,$$

here B_p are the Bernoullian numbers.

The quantity to evaluate is, according to (2.12)

$$I = \sum_{l=-\infty}^{\infty} \frac{i_0\,(l-\varphi)}{e^{\beta\epsilon_0(l-\varphi)^2-\beta\mu}+1}, \qquad (2.14)$$

here $i_0 = \hbar/2\pi mR^2$ and $\epsilon_0 = \hbar^2/2mR^2$. β is $1/k_BT$. We suggest to expand (2.14) in the reduced flux φ, and to use the Euler-Maclaurin formula separately at each order of this perturbation theory. Of course the temperature should be kept finite to have a well-defined perturbation theory at all - the current is a discontinuous function of φ at $T = 0$. Now, according to the Byers-Yang theorems, the persistent current, being the φ derivative of the grand canonical potential, is an odd function of the reduced flux. Hence the perturbation expansion of I will only contain terms with odd powers of φ: $I = I_1\varphi + I_3\varphi^3 + \ldots$. The first order in φ is found to be

$$\begin{aligned} I_1 &= \sum_{l=-\infty}^{\infty}\left(-\frac{i_0}{2\epsilon_0}E_l''f\,(E_l) - \frac{i_0}{2\epsilon_0}(E_l')^2 f\,'(E_l)\right) \\ &= \sum_{l=-\infty}^{\infty}\left(\frac{-i_0}{e^{\beta\epsilon_0 l^2-\beta\mu}+1} + \frac{2\beta\epsilon_0 i_0 l^2 e^{\beta\epsilon_0 l^2-\beta\mu}}{\left(e^{\beta\epsilon_0 l^2-\beta\mu}+1\right)^2}\right), \end{aligned} \qquad (2.15)$$

and the third order is

$$I_3 = \sum_{l=-\infty}^{\infty} -\frac{i_0}{4\epsilon_0}(E_l'')^2 f\,'(E_l) - \frac{i_0}{2\epsilon_0}E_l''(E_l')^2 f\,''(E_l) - \frac{i_0}{12\epsilon_0}(E_l')^4 f\,'''(E_l), \qquad (2.16)$$

here E_l, E_l', E_l'' are the energy, its first and second derivatives with respect to the reduced flux φ, evaluated at $\varphi = 0$. We start with the first order, which can be rewritten in a form suitable for the application of the Euler-Maclaurin formula

$$I_1 = \frac{-i_0}{e^{-\beta\mu}+1} + \sum_{l=1}^{\infty}\frac{-2i_0}{e^{\beta\epsilon_0 l^2-\beta\mu}+1} + \sum_{l=1}^{\infty}\frac{4\beta\epsilon_0 i_0 l^2 e^{\beta\epsilon_0 l^2-\beta\mu}}{\left(e^{\beta\epsilon_0 l^2-\beta\mu}+1\right)^2}. \qquad (2.17)$$

Using now (2.14) to calculate the first sum in this formula, we will find that the term $-(1/2)F(0)$ is exactly canceled by the first term of (2.17), where $F(x) = 1/\exp(\beta\epsilon_0 x^2 - \beta\mu)$. All the other terms in the series, except the one given by the integral, vanish. The only non-zero contribution to the second sum in (2.17) may

also result from the first term of the Euler-Maclaurin series. Therefore to first order in φ, the persistent current in the one-dimensional ring is asymptotically equal to

$$I_1 \sim \int_0^\infty dx \frac{-2i_0}{e^{\beta\epsilon_0 x^2-\beta\mu}+1} + \int_0^\infty dx \frac{4\beta\epsilon_0 i_0 x^2 e^{\beta\epsilon_0 x^2-\beta\mu}}{\left(e^{\beta\epsilon_0 x^2-\beta\mu}+1\right)^2}. \tag{2.18}$$

It is sufficient to calculate the first integral, since the second one is proportional to the derivative of the first with respect to ϵ_0. We will digress now to evaluate it. Remember that $\alpha = \beta\mu$ is a very large parameter, hence the expansion of the first integral in $1/\alpha$ would suffice. The integral is separated into two parts

$$\int_0^\infty dx \frac{1}{e^{x^2-\alpha}+1} = \int_0^{\sqrt{\alpha}} dx \frac{1}{e^{x^2-\alpha}+1} + \int_{\sqrt{\alpha}}^\infty dx \frac{1}{e^{x^2-\alpha}+1}. \tag{2.19}$$

The first term is transformed expanding the integrand into the geometric series

$$\int_0^{\sqrt{\alpha}} dx \frac{1}{e^{x^2-\alpha}+1} = \int_0^{\sqrt{\alpha}} dx\left(1 - e^{x^2-\alpha} + e^{2\left(x^2-\alpha\right)} - \dots\right)$$

$$= \sqrt{\alpha} - e^{-\alpha}\int_0^{\sqrt{\alpha}} e^{x^2} dx + \frac{1}{\sqrt{2}} e^{-2\alpha}\int_0^{\sqrt{2\alpha}} e^{x^2} dx - \dots.$$

The resulting expression is the series of the error functions, for which asymptotic expansions for large arguments exist and can be found among others in [8]. Using these asymptotic formulas, the large α behavior of the first term turns out to be

$$\int_0^{\sqrt{\alpha}} dx \frac{1}{e^{x^2-\alpha}+1} \sim \sqrt{\alpha} - \frac{1}{2\sqrt{\alpha}}\ln 2 - \frac{\pi^2}{48\alpha^{3/2}} + \dots. \tag{2.20}$$

The second part in (2.19) is transformed multiplying and dividing the integrand by $\exp(-x^2+\alpha)$. Afterwards it is also expanded into geometric series, now involving only the complementary error functions

$$\int_{\sqrt{\alpha}}^\infty dx \frac{1}{e^{x^2-\alpha}+1} = \int_{\sqrt{\alpha}}^\infty dx \frac{e^{-x^2+\alpha}}{e^{-x^2+\alpha}+1}$$

$$= \int_{\sqrt{\alpha}}^\infty dx\left(e^{-x^2+\alpha} - e^{-2\left(x^2-\alpha\right)} + e^{-3\left(x^2-\alpha\right)} - \dots\right)$$

$$= e^{\alpha}\int_{\sqrt{\alpha}}^\infty dx e^{-x^2} - \frac{1}{\sqrt{2}} e^{2\alpha}\int_{\sqrt{2\alpha}}^\infty dx e^{-x^2} + \dots.$$

Once more using the asymptotic expansion of the large argument complementary error function, the second term is asymptotically equivalent to

$$\int_{\sqrt{\alpha}}^\infty dx \frac{1}{e^{x^2-\alpha}+1} \sim \frac{1}{2\sqrt{\alpha}}\left(\ln 2 - \frac{\pi^2}{24\alpha} + \dots\right). \tag{2.21}$$

Adding (2.20) and (2.21), the leading asymptotic term of the whole integral is seen to be

$$\int_0^\infty dx \frac{1}{e^{x^2-\alpha}+1} \sim \sqrt{\alpha} - \frac{\pi^2}{24\alpha^{3/2}} + \cdots. \tag{2.22}$$

Coming back now to the two integrals in the expression of the persistent current (2.18), the first one is easily found to behave as

$$\int_0^\infty dx \frac{-2i_0}{e^{\beta\epsilon_0 x^2-\beta\mu}+1} \sim -2i_0\sqrt{\frac{\mu}{\epsilon_0}} + \frac{\pi^2 i_0}{12\beta^2\epsilon_0^{1/2}\mu^{3/2}} - \cdots. \tag{2.23}$$

The second integral, as was already mentioned is proportional to the derivative with respect to ϵ_0 of the first one. Therefore its asymptotic form is readily derived from (2.23)

$$\int_0^\infty dx \frac{4\beta\epsilon_0 i_0 x^2 e^{\beta\epsilon_0 x^2-\beta\mu}}{\left(e^{\beta\epsilon_0 x^2-\beta\mu}+1\right)^2} \sim 2i_0\sqrt{\frac{\mu}{\epsilon_0}} - \frac{\pi^2 i_0}{12\beta^2\epsilon_0^{1/2}\mu^{3/2}} + \cdots. \tag{2.24}$$

As a result, first order in φ, the total current, I_1 is asymptotically zero - the two terms forming it are large, but have opposite signs.

In the third order (2.16) all three terms can be computed according to the same pattern. Consider for instance the first term

$$-\sum_{l=-\infty}^{\infty} \frac{i_0}{4\epsilon_0}(E_l'')^2 f'(E_l) = \sum_{l=-\infty}^{\infty} \frac{\beta\epsilon_0 i_0 e^{\beta\epsilon_0 l^2-\beta\mu}}{\left(e^{\beta\epsilon_0 l^2-\beta\mu}+1\right)^2}.$$

It is not difficult to get convinced that from all the Euler-Maclaurin series only the first term is non-zero (here again we separate $l=0$ from the rest of the sum, and this term is canceled out by the second term in the summation formula). Therefore we are left with

$$-\sum_{l=-\infty}^{\infty} \frac{i_0}{4\epsilon_0}(E_l'')^2 f'(E_l) \sim \int_0^\infty dx \frac{2\beta\epsilon_0 i_0 e^{\beta\epsilon_0 x^2-\beta\mu}}{\left(e^{\beta\epsilon_0 x^2-\beta\mu}+1\right)^2}. \tag{2.25}$$

This integral is also a close relative of (2.19). Namely, it is proportional to the derivative of (2.23) with respect to μ. More precisely

$$-\sum_{l=-\infty}^{\infty} \frac{i_0}{4\epsilon_0}(E_l'')^2 f'(E_l) \sim i_0\sqrt{\frac{\epsilon_0}{\mu}} - \frac{3\pi^2 i_0 \epsilon_0^{1/2}}{24\beta^2\mu^{5/2}} + \cdots. \tag{2.26}$$

Another two terms are of the same order, the second twice as large as the first with the opposite sign, the third one equal to the first, and all three together give zero average persistent current again. Our conclusion is hence that the persistent current averaged over the different values of chemical potential is zero up to third order in perturbation in the reduced flux.

To further substantiate these conclusions, we would like to show that the leading behavior of different orders of the perturbation can be inferred from few very simple,

though less rigorous arguments. We know a posteriori that the leading asymptotic expressions to be found are temperature independent. Therefore we assume that $T = 0$. The first order of the persistent current consists of the two parts (2.15) - diamagnetic and paramagnetic, I_1^d and I_1^p respectively. The diamagnetic part, to remind, is

$$I_1^d = \sum_{l=-\infty}^{\infty} -\frac{i_0}{2\epsilon_0} E_l'' f\left(E_l\right). \tag{2.27}$$

The Fermi-Dirac distribution for $T = 0$ allows only for states with energies less than the chemical potential in the sum (2.27). At zero flux and zero temperature the chemical potential fixes the number of particles N. Let l_F be the "Fermi level", defined by $\mu = \epsilon_0 l_F^2$. Then because of degeneracy $N = 2l_F$. Since $E_l'' = 2\epsilon_0$, the sum of the Fermi-Dirac distribution is equal to the number of particles and the previous result (2.23) follows

$$I_1^d \sim -i_0 N = -2i_0\sqrt{\frac{\mu}{\epsilon_0}}.$$

The paramagnetic term involves the derivative of the Fermi-Dirac distribution

$$I_1^p = -\sum_{l=-\infty}^{\infty} \frac{i_0}{2\epsilon_0}(E_l')^2 f'\left(E_l\right). \tag{2.28}$$

Strictly speaking, because this derivative is proportional to a delta function, the expression (2.28) is not well defined. We claim that instead of a sum over the discrete states, an integral over the continuous spectrum appears. This integral is then equal to the integrand evaluated at the chemical potential times the density of states there. The density of states can be approximated by the degeneracy divided by the level spacing Δ at the chemical potential. Because $E_l' = -2l\epsilon_0$ and $\Delta = 2l_F\epsilon_0$

$$I_1^p \sim 4i_0\epsilon_0 l_F^2/\Delta = 2i_0\sqrt{\frac{\mu}{\epsilon_0}}.$$

Indeed the paramagnetic current is of the same magnitude as the diamagnetic one, but of opposite sign. The diamagnetic part of the persistent current is the sum of the small second derivative of the energy over all the occupied states, whereas the paramagnetic part is proportional to the square of the large first derivative of the energy taken only at the chemical potential (only the level that crosses the Fermi surface contributes).

The cancelation of diamagnetic and paramagnetic parts of the current has two different causes: the first is the averaging over the energies itself, as before doing it the current was evidently finite; the second one is the special form of the energies, for it is probable that if the energies would have a different φ dependence, the current would not cancel out.

2.3 A one-dimensional ring with impurities.

It seems to be a matter of consensus that the grand-canonical persistent current vanishes after disorder averaging. One possible calculation demonstrating this is

given in [9], where the authors starting from (2.12) transform it to the following form

$$I = \int_{-\infty}^{\infty} \frac{dE}{2\pi i} \sum_{l=-\infty}^{\infty} f(E) \left(\frac{i_0(l-\varphi)}{E - \epsilon_0(l-\varphi)^2 + \frac{i\hbar}{2\tau}} - \text{c.c.} \right). \tag{2.29}$$

This would be the current in a one-dimensional clean ring, if the poles of the integrand in (2.29) were placed on the real axis in the complex E plane. However, the poles in this case are removed by $\hbar/2\tau$ from the real axis, thus smearing the states over this energy scale. Such a smoothing of the spectrum gives smooth, averaged quantities and is a well-known method to calculate the asymptotic expansion of the density of states for the large energies [10]. Therefore the method to find the average grand-canonical persistent current suggested in [9] is nothing but another way of smoothing the current in the clean ring over the energy. This is exactly what we did in the previous section. However is the average all what the disorder does? Are the properties of the spectrum itself unimportant? This could hardly be the case, because as is clear the disorder affects the energy levels by removing the degeneracies and inducing a level statistics which substantially differs from that of the clean system. We suggest then to consider a one-dimensional ring with impurities, still an integrable system, but possessing a spectrum different from (2.8), to find its average current and check if it is also zero.

The simplest thing that comes to mind is a ring with one impurity represented by a Dirac delta-function, in other words the Kronig-Penney model. The corresponding Schrödinger equation is

$$-\frac{\hbar^2}{2mR^2} \left(\frac{\partial}{\partial\theta} - i\frac{\varphi}{2\pi} \right)^2 \psi + (V_0\delta(\theta) - E)\psi = 0. \tag{2.30}$$

This model is the simplest possessing a conduction band and forbidden gap structure. In our case the bands correspond to the energy levels depending on the reduced flux (note that the reduced flux here is defined with $\hbar$, instead of h, therefore its unit is 2π). The equation can be derived that leads to those energy levels [11]

$$\frac{P}{\lambda}\sin\lambda + \cos\lambda = \cos\varphi, \tag{2.31}$$

here $\lambda^2 = E/\epsilon_0$ and $P = V_0/2\epsilon_0$. This is a transcendental equation and it can not be solved to give an analytic expression for the energy. However to do the required smoothing of the persistent current to the leading order, only very large energies are relevant. Our goal now is to do the perturbation in φ for the total persistent current up to the third order and then smooth over the energy the exact expressions. To that purpose, we need the expansion of the energies up to the fourth order in the reduced flux with the sufficient accuracy.

The left-hand side of (2.31) is an even function of λ, therefore we can consider only positive λ's. First take $\varphi = 0$. Immediately we see that $\lambda_l = 2\pi l$, $l \neq 0$ solve (2.31). In addition to these, there is another set of solutions, given asymptotically by

$$\tilde{\lambda}_l = 2\pi l + P/\pi l - \frac{P^2}{2(\pi l)^3}\left(1 + \frac{P}{6}\right) + \frac{P^3}{4(\pi l)^5}\left(1 + \frac{P}{3} + \frac{P^2}{40}\right) + \mathrm{O}(\frac{1}{l^7}), \tag{2.32}$$

here we think of l being the large parameter and solve (2.31) order by order. For the sake of consistency, P should be taken as a small number. The first derivatives at $\varphi = 0$ of both λ_l and $\tilde{\lambda}_l$ are seen to vanish (in fact all odd derivatives at $\varphi = 0$ are zero). For our purposes we will need the second and fourth derivatives of both sets of energies. For the first set, both derivatives can be calculated exactly

$$\begin{aligned} \lambda_l'' &= -2\pi l/P, \\ \lambda_l^{\rm iv} &= \frac{2\pi l}{P}\left(3\left(\frac{2\pi l}{P}\right)^2 + 6/P + 1\right), \end{aligned}$$

here the derivatives are taken at zero flux. For the second set both derivatives can be found again expanding the equation (2.31) for large l's, order by order. After a somewhat lengthy calculation, using (2.32), we obtain

$$\begin{aligned} \tilde{\lambda}_l'' &= 2\pi l/P + \frac{P}{2(\pi l)^3}\left(3 + P + P^2/20\right) + \mathrm{O}(1/l^5), \\ \tilde{\lambda}_l^{\rm iv} &= -\frac{2\pi l}{P}\left(3\left(\frac{2\pi l}{P}\right)^2 + \frac{6}{P} + 1\right) - \frac{6}{\pi l}\left(\frac{6}{P} + 2 + \frac{3P}{20}\right) + \mathrm{O}(\frac{1}{l^3}). \end{aligned}$$

The corresponding energies up to the fourth order in φ are then

$$\begin{aligned} E_l(\varphi)/\epsilon_0 &= (2\pi l)^2 - \frac{(2\pi l\varphi)^2}{P} + \frac{(2\pi l)^2}{12P}\left(3\left(\frac{2\pi l}{P}\right)^2 + \frac{9}{P} + 1\right)\varphi^4 \\ \tilde{E}_l(\varphi)/\epsilon_0 &= (2\pi l)^2 + 4P - \left(\frac{P}{\pi l}\right)^2(1 + \frac{P}{3}) + \frac{(2\pi l\varphi)^2}{P} + 2\varphi^2 - \\ &- \frac{(2\pi l)^2}{12P}\left(3\left(\frac{2\pi l}{P}\right)^2 + \frac{9}{P} + 1\right)\varphi^4 - (\frac{6}{P} + 2 + \frac{3P}{20})\varphi^4 + \cdots, \end{aligned} \tag{2.33}$$

here the energies of the second set contain also lower powers of $1/l$, not relevant to this discussion. The total persistent current in the grand-canonical ensemble is according to (2.12)

$$I = -\frac{1}{h}\sum_{l=1}^{\infty}\left(f(E_l(\varphi))\frac{\partial E_l(\varphi)}{\partial\varphi} + f(\tilde{E}_l(\varphi))\frac{\partial\tilde{E}_l(\varphi)}{\partial\varphi}\right). \tag{2.34}$$

The first order term in the small φ expansion of the persistent current is

$$I_1 = -\frac{1}{h}\sum_{l=1}^{\infty}\left(f(E_l)E_l'' + f(\tilde{E}_l)\tilde{E}_l''\right), \tag{2.35}$$

here again the energies and their derivatives are to be taken at zero flux, from (2.33). The problem however is that the second equation in (2.33) is only valid for large energies (large l's), hence we do not possess the analytic expression even for the first term in φ expansion, I_1. This prevents us from using the Euler-Maclaurin formula to smooth the current over the spectrum. We are left with somewhat loose arguments

to evaluate the leading term of the total persistent current, which we used in the previous section for the case of the clean ring. Substituting the actual energies and derivatives into (2.35), we have for the large energies

$$\begin{aligned} I_1 &\sim i_0 \sum_{l=1}^{\infty} f\left(\epsilon_0 (2\pi l)^2\right) \frac{8}{P} (\pi l)^2 - i_0 \sum_{l=1}^{\infty} f\left(\epsilon_0 \left((2\pi l)^2 + 4P\right)\right) \left(\frac{8}{P} (\pi l)^2 + 4\right) \\ &\sim -i_0 \sum_{l=1}^{\infty} f\left(\epsilon_0 (2\pi l)^2\right) 4 - f'\left(\epsilon_0 (2\pi l)^2\right) 4P\epsilon_0 \left(\frac{8}{P} (\pi l)^2\right). \end{aligned} \tag{2.36}$$

The two terms in (2.36) can be evaluated taking the temperature to be zero. The first term is proportional to the number of particles in the ring, the second one should be treated exactly like (2.28) - considering the integral over the energies instead of the sum. These arguments give the following result for the leading term in the asymptotic expansion of the first order in φ of the total persistent current in the one-impurity ring

$$I_1 \sim -\frac{2i_0}{\pi}\sqrt{\frac{\mu}{\epsilon_0}} + \frac{2i_0}{\pi}\sqrt{\frac{\mu}{\epsilon_0}} = 0.$$

Therefore as in the case of the clean one-dimensional ring, the first order in the flux contribution to the current vanishes. We go to the third order now, which for this model is according to (2.34)

$$I_3 = -\frac{1}{h} \sum_{l=1}^{\infty} \left(f(E_l) \frac{E_l^{\mathrm{iv}}}{6} + f(\tilde{E}_l) \frac{\tilde{E}_l^{\mathrm{iv}}}{6} + f'(E_l) \frac{(E_l'')^2}{2} + f'(\tilde{E}_l) \frac{\left(\tilde{E}_l''\right)^2}{2} \right).$$

Substituting the actual energies (2.33) into this equation, we find the following, quite tedious expression for I_3, involving terms with different powers of the large parameter l

$$\begin{aligned} I_3 \sim & -i_0 \sum_{l=1}^{\infty} f\left(\epsilon_0 (2\pi l)^2\right) \frac{(2\pi l)^2}{3P} \left(3\left(\frac{2\pi l}{P}\right)^2 + \frac{9}{P} + 1\right) \\ & + i_0 \sum_{l=1}^{\infty} f\left(\epsilon_0 \left((2\pi l)^2 + 4P - \left(\frac{P}{\pi l}\right)^2 (1 + \frac{P}{3})\right)\right) \frac{(2\pi l)^2}{3P} \left(3\left(\frac{2\pi l}{P}\right)^2 + \frac{9}{P} + 1\right) \\ & + i_0 \sum_{l=1}^{\infty} \left(f\left(\epsilon_0 (2\pi l)^2\right) (\frac{6}{P} + 2 + \frac{3P}{20}) 4 - f'\left(\epsilon_0 \left((2\pi l)^2 + 4P\right)\right) \frac{2(2\pi l)^4 \epsilon_0}{P^2} \right) \\ & - i_0 \sum_{l=1}^{\infty} \left(f'\left(\epsilon_0 (2\pi l)^2\right) \frac{8(2\pi l)^2 \epsilon_0}{P} + f'\left(\epsilon_0 (2\pi l)^2\right) \frac{2(2\pi l)^4 \epsilon_0}{P^2} \right). \end{aligned}$$

This expression can be simplified by expanding the arguments of the Fermi-Dirac functions in $1/l$, then quite a few cancelations occur and a simple formula remains

$$I_3 \sim i_0 \sum_{l=1}^{\infty} \left(f\left(\epsilon_0 (2\pi l)^2\right) (\frac{6}{P} + 2 + \frac{3P}{20}) 4 + f'\left(\epsilon_0 (2\pi l)^2\right) \frac{4(2\pi l)^2 \epsilon_0}{3} \left(\frac{9}{P} + 1\right) \right)$$

$$-i_0\sum_{l=1}^{\infty}\left(f'\left(\epsilon_0(2\pi l)^2\right)\frac{4(2\pi l)^2\epsilon_0}{P}(1+\frac{P}{3})+f'\left(\epsilon_0(2\pi l)^2\right)\frac{8(2\pi l)^2\epsilon_0}{P}\right)$$
$$= i_0\sum_{l=1}^{\infty}f\left(\epsilon_0(2\pi l)^2\right)(\frac{6}{P}+2+\frac{3P}{20})4. \tag{2.37}$$

The asymptotic analysis using the Euler-Maclaurin summation formula now can be applied on the expression in (2.37). Using the expansion (2.22), the following asymptotic result is obtained for I_3

$$I_3 \sim \frac{2i_0}{\pi}\sqrt{\frac{\mu}{\epsilon_0}}\frac{6}{P}-\frac{i_0\pi}{12\beta^2\epsilon_0^{1/2}\mu^{3/2}}\frac{6}{P}+\cdots. \tag{2.38}$$

The result (2.38) is non-perturbative, in the sense that taking the strength of the delta-like impurity P to be zero gives a diverging expression. This is due to the nature of the curvature at zero flux, which becomes greater, when P is reduced. An interesting temperature dependence of (2.38) should be noted - the leading term is temperature independent, the correction increases with the temperature, reducing the current quadratically. The two terms become comparable at an enormous temperature $\beta\mu = 1$ (practically this temperature is not relevant, being higher than the melting temperature of the ring).

We obtained here a non-zero (in fact paramagnetic) contribution in the third order term of the reduced flux expansion of the current, illustrating the point that the smoothed persistent current is definitely sensitive to the properties of the spectrum. Thus by smoothing the current over the spectrum of a clean system one could miss the important effect the disorder has on the energy levels, which at the end could give rise to a non-zero average current. Under the impression of these arguments one would be tempted to think that each time the degeneracy of the clean spectrum is removed by opening gaps, a finite average current should turn out as a result of the smoothing. Things are however more subtle than that as we show now considering a model system possessing finite gaps in its spectrum, but for which the average current nevertheless vanishes.

Consider a particle moving in a one-dimensional ring with a singular potential which obeys the following Schrödinger equation

$$-\frac{\hbar^2}{2mR^2}\left(\frac{\partial}{\partial\theta}-i\frac{\varphi}{2\pi}\right)^2\psi-\left(\frac{V_0}{\sin^2(\theta/2)}+E\right)\psi=0. \tag{2.39}$$

This model was solved by F. L. Scarf [12] in the context of periodic potential theory. It is more convenient to represent the equation (2.39) in different variables

$$\left(\frac{\partial}{\partial\theta_1}-i\frac{\varphi_1}{2\pi}\right)^2\psi+\left(\frac{1/4-s^2}{\sin^2(\theta_1)}+\lambda_1^2\right)\psi=0, \tag{2.40}$$

where $\theta_1 = \theta/2$, $\varphi_1 = 2\varphi$, $\lambda_1 = 2\lambda$ and $1/4 - s^2 = 4V_0/\epsilon_0$. In the sequel we shall drop the subscripts in the notations, hoping that this will not lead to confusion. The

energies as functions of the reduced flux are found from the equation first deduced in [12]

$$\lambda = \arccos\left(\sin \pi s \cos \varphi\right). \tag{2.41}$$

Inverse cosine is a multivalued function, its different branches giving rise to energy levels. At $\varphi = 0$ these are $\lambda_l = \pi\left(1/2 - s + 2l\right)$, when l here is allowed to be any integer (positive or negative), in contrast with the Kronig-Penney model, where it had to be positive. As for the Kronig-Penney model, the odd derivatives of λ in the reduced flux at $\varphi = 0$ vanish. The second and fourth derivatives are easily calculated from (2.41) and turn out to be l-independent

$$\begin{aligned} \lambda_l'' &= \tan \pi s \\ \lambda_l^{\mathrm{iv}} &= -\left(\tan \pi s + 3\tan^3 \pi s\right). \end{aligned} \tag{2.42}$$

The corresponding energies up to the fourth order in φ follow from (2.42)

$$\begin{aligned} E_l(\varphi) &= \frac{\epsilon_0}{4}(\pi^2\left(1/2 - s + 2l\right)^2 + \pi\left(1/2 - s + 2l\right)(\tan \pi s)\varphi^2 \\ &+\frac{1}{4}(\tan \pi s)^2\varphi^4 - \frac{\pi}{12}(\tan \pi s + 3\tan^3 \pi s)\left(1/2 - s + 2l\right)\varphi^4). \end{aligned} \tag{2.43}$$

We are ready now to calculate the first and third orders of the persistent current in φ, which are given by

$$I_1 = -\frac{1}{h}\sum_{l=-\infty}^{\infty} f(E_l)E_l'', \tag{2.44}$$

$$I_3 = -\frac{1}{h}\sum_{l=-\infty}^{\infty}\left(f(E_l)\frac{E_l^{\mathrm{iv}}}{6} + f'(E_l)\frac{(E_l'')^2}{2}\right). \tag{2.45}$$

The explicit expression for the first order term is obtained inserting the relevant information from (2.43) to the general equation (2.44)

$$I_1 = -\frac{i_0}{8}\sum_{l=-\infty}^{\infty} f\left(\frac{\epsilon_0\pi^2}{4}\left(1/2 - s + 2l\right)^2\right)\pi\left(1/2 - s + 2l\right)(\tan \pi s). \tag{2.46}$$

We have a closed and simple enough function of l in the sum (2.46) to smooth it over the spectrum and to apply the Euler-Maclaurin summation formula will be applicable. The calculation is very similar to that performed for the one-dimensional clean ring. We split the sum into three parts - positive, zero and negative l's, and after an inspection of the general formula (2.14), only two integrals corresponding to positive and negative l parts are seen to give substantial contributions

$$I_1 \sim -\frac{i_0}{8}\left(\int_0^{\infty} dx \frac{\pi\left(1/2 - s + 2x\right)(\tan \pi s)}{e^{\beta\widetilde{\epsilon}_0(1/2-s+2x)^2 - \beta\mu} + 1} + \int_0^{\infty} dx \frac{\pi\left(1/2 - s - 2x\right)(\tan \pi s)}{e^{\beta\widetilde{\epsilon}_0(1/2-s-2x)^2 - \beta\mu} + 1}\right), \tag{2.47}$$

here $\widetilde{\epsilon}_0 = \epsilon_0\pi^2/4$. However it is easy to get convinced that the expression in the brackets of the left-hand side of (2.47) is zero. Hence as for the free ring and for the

Kronig-Penney model, the first order in the reduced flux of the persistent current vanishes.

It is convenient to separate the third order term of the persistent current (2.45) into two parts in the following way

$$\begin{aligned} I_3^{(1)} = & \quad \frac{i_0}{12} \sum_{l=-\infty}^{\infty} f\left(\tilde{\epsilon}_0 (1/2 - s + 2l)^2\right) \pi (1/2 - s + 2l) (\tan \pi s + 3 \tan^3 \pi s), \\ I_3^{(2)} = & \quad -\frac{i_0}{4} \sum_{l=-\infty}^{\infty} f\left(\tilde{\epsilon}_0 (1/2 - s + 2l)^2\right) \tan^2 \pi s \\ & -\frac{i_0}{4} \sum_{l=-\infty}^{\infty} f'\left(\tilde{\epsilon}_0 (1/2 - s + 2l)^2\right) 2\tilde{\epsilon}_0 \left((1/2 - s + 2l)(\tan \pi s)\right)^2, \end{aligned} \quad (2.48)$$

where the third order current $I_3 = I_3^{(1)} + I_3^{(2)}$. The first part is proportional to the first order contribution (2.46) and therefore is zero asymptotically. The second part after a similar line of arguments as the one that led to (2.47), is seen to be asymptotically equal to

$$I_3^{(2)} \sim -\frac{i_0}{4} \int_0^{\infty} dx \frac{(\tan \pi s)^2}{e^{\beta \tilde{\epsilon}_0 x^2 - \beta\mu} + 1} + \frac{i_0}{4} \int_0^{\infty} dx \frac{2\beta \tilde{\epsilon}_0 x^2 (\tan \pi s)^2}{\left(e^{\beta \tilde{\epsilon}_0 x^2 - \beta\mu} + 1\right)^2} e^{\beta \tilde{\epsilon}_0 x^2 - \beta\mu}. \quad (2.49)$$

The first integral is proportional to the integral in (2.19). Using its asymptotic expansion valid for large $\beta\mu$ (2.22), we obtain for the leading term

$$\frac{i_0}{4} \int_0^{\infty} dx \frac{(\tan \pi s)^2}{e^{\beta \tilde{\epsilon}_0 x^2 - \beta\mu} + 1} \sim \frac{i_0}{4} (\tan \pi s)^2 \sqrt{\frac{\mu}{\tilde{\epsilon}_0}}.$$

The second integral in (2.49) is proportional to the derivative of the first one with respect to $\tilde{\epsilon}_0$, and has the following asymptotic form

$$\frac{i_0}{4} \int_0^{\infty} dx \frac{2\beta \tilde{\epsilon}_0 x^2 (\tan \pi s)^2}{\left(e^{\beta \tilde{\epsilon}_0 x^2 - \beta\mu} + 1\right)^2} e^{\beta \tilde{\epsilon}_0 x^2 - \beta\mu} \sim \frac{i_0}{4} (\tan \pi s)^2 \sqrt{\frac{\mu}{\tilde{\epsilon}_0}}.$$

As a result the third order in φ of the persistent current is zero in the Scarf's potential, thus providing an example of a system with a non-degenerate spectrum, but vanishing smoothed current. The situation here is unlike that in the Kronig-Penney model, where the current was finite due to repulsion of the neighboring levels. It would be extremely desirable to understand the general principles causing the smoothed persistent current to be zero or finite.

2.4 Disordered many-channel ring.

A one-dimensional ring is not a particularly relevant system experimentally (though an experiment was reported on almost one-dimensional ring, fabricated in semiconductor based structures [13]). The two important experiments [14, 15], where the

persistent current was measured, were performed on thick metallic rings. For example in the experiments of the IBM group [15], the magnetization of three different gold loops was measured. Two of the loops were rings of diameter 2.4 and 4.0 μm, the linewidths of the loops was $\simeq$ 90 nm and the thickness of the Au films $\simeq$ 60 nm. The number of transverse channels in such a ring can be estimated to be approximately 23000. An oscillatory component in the magnetic response was measured, oscillating with a fundamental period Φ_0. The amplitude of this oscillatory current was found to correspond to a persistent current at $T = 0$ of order $(0.3-2.0)ev_F/2\pi R$ (in our notation this current corresponds to $i_0\sqrt{\mu/\epsilon_0}$). Such a value proved to be a theoretical challenge, and our work is another attempt in that direction.

We suggest continuing the study of the persistent current along similar lines as in the case of one-dimensional systems. Namely, we expand the persistent current in the reduced flux, and smooth the result at each order over the energies. Since the ring has a width, which is large compared to the Fermi wavelength of the electrons, one is tempted to use the diagrammatic technique [16, 17] to average over the impurities, based on the Green's functions formalism. As we hope to show later in this section, this route has its perils, because the method is only applicable for extended systems, whereas it is crucial in calculating the smoothed current to take into account the statistics of the energy spectrum, which is possible only by considering a truly finite-size system. In fact the calculations giving zero disorder average of the current, are found to be equivalent to the smoothing over the spectrum of the clean ring presented in the second section.

Nevertheless, we will present now the perturbation theory for the persistent current in terms of Green's functions. We shall work with the Hamiltonian (2.7), which represents the periodic (and disordered) potential problem. The Hamiltonian H can be separated into two parts - an unperturbed one, H_0 , which does not depend on the reduced flux, and the perturbation H_1, containing all the dependence on φ

$$\begin{aligned} H_0 &= -\frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}+\frac{\partial^2}{\partial z^2}\right)+V(\mathbf{r}), \\ H_1 &= -\frac{\hbar}{mR}p_x\varphi+\epsilon_0\varphi^2. \end{aligned} \tag{2.50}$$

We define the retarded and advanced Green's operators, G^R and G^A respectively, in the usual way

$$G^{R,A}(E) = \frac{1}{E - H \pm i\eta}. \tag{2.51}$$

Then, the persistent current is given by

$$I = -\int_{-\infty}^{\infty}\frac{dE}{2\pi hi}\mathrm{Tr}\, f(E)\left(G^A(E)-G^R(E)\right)\frac{\partial H_1}{\partial\varphi}, \tag{2.52}$$

where the integration is in the complex E plane, along the contour closed in the upper halfplane. The formal perturbation series in φ is obtained, by expanding the Green's function with respect to the perturbed part H_1 of the Hamiltonian

$$G^{R,A}(E) = G_0^{R,A}(E) + G_0^{R,A}(E)H_1G_0^{R,A}(E) + \cdots, \tag{2.53}$$

here $G_0^{R,A}(E)$ is the unperturbed Green's operator, $G_0^{R,A}(E) = 1/(E - H_0 \pm i\eta)$. Using the expansion (2.53) it is a simple matter to write down the different orders of the perturbation theory in the reduced flux for the current. For example, the first order term is

$$\begin{aligned} I_1 &= -i_0 \int_{-\infty}^{\infty} \frac{dE}{2\pi i} \mathrm{Tr}\, f(E) \left(G_0^A(E) - G_0^R(E) \right) \\ &\quad - \frac{i_0}{2m} \int_{-\infty}^{\infty} \frac{dE}{\pi i} \mathrm{Tr}\, f(E) \left(G_0^A(E) p_x G_0^A(E) p_x - \text{c.c.} \right). \end{aligned} \tag{2.54}$$

In this form, we can average (2.54) over the disorder. To this end, the plane wave basis is used, and the disorder averaged Green's functions can be shown to be [16, 17]

$$\left\langle G_0^{R,A}(E) \right\rangle = \frac{1}{E - \frac{p^2}{2m} \pm \frac{i\hbar}{2\tau}}, \tag{2.55}$$

the brackets here indicate the average over the disorder, and $\mathbf{p}$ is the momentum. We insert now these Green's functions into (2.54), obtaining the disorder averaged current $\langle I_1 \rangle$

$$\begin{aligned} \langle I_1 \rangle &= -i_0 \int_{-\infty}^{\infty} \frac{dE}{\pi i} \int \frac{V d\mathbf{p}}{(2\pi\hbar)^3} f(E) \left(\frac{1/2}{E - \frac{p^2}{2m} - \frac{i\hbar}{2\tau}} - \text{c.c.} \right) \\ &\quad -i_0 \int_{-\infty}^{\infty} \frac{dE}{\pi i} \int \frac{V d\mathbf{p}}{(2\pi\hbar)^3} f(E) \left(\frac{p_x^2/2m}{\left(E - \frac{p^2}{2m} - \frac{i\hbar}{2\tau} \right)^2} - \text{c.c.} \right) \\ &= -i_0 \int_{-\infty}^{\infty} \frac{dE}{\pi i} \int \frac{V d\mathbf{p}}{(2\pi\hbar)^3} f(E) \left(\frac{1/2}{E - \frac{p^2}{2m} - \frac{i\hbar}{2\tau}} - \text{c.c.} \right) \\ &\quad -i_0 \int_{-\infty}^{\infty} \frac{dE}{\pi i} \int \frac{V d\mathbf{p}}{(2\pi\hbar)^3} f'(E) \left(\frac{p_x^2/2m}{E - \frac{p^2}{2m} - \frac{i\hbar}{2\tau}} - \text{c.c.} \right) \end{aligned} \tag{2.56}$$

The second term here has been integrated by parts; V is the volume of the system. This result should be compared with the first order of the persistent current in the one-dimensional clean ring (2.15), the similarity between these two formulas is clear. Now we will calculate the integrals in (2.56) and show that smoothing over the spectrum in the clean one-dimensional ring and doing the disorder average in this extended three-dimensional system yield the same results and are basically equivalent, i.e. $\langle I \rangle = 0$. The integration of (2.56) is particularly simple for $T = 0$. The first, diamagnetic term in $\langle I_1 \rangle$ is equal to $-i_0 N$, where N is the total number of the electrons in the system. The paramagnetic term is evaluated recalling that at $T = 0$ the derivative of the Fermi-Dirac distribution is up to a sign a delta function at the Fermi energy E_F

$$\langle I_1 \rangle^p = 2 i_0 V \rho(\mu) \mu \frac{1}{3}.$$

Here $\rho(\mu)$ is the density of levels at the Fermi energy, which according to [4] is connected to the density of the particles in the system via $\rho(\mu) = 3N/2V\mu$. Therefore the paramagnetic part is equal in magnitude to the diamagnetic part of the current, but opposite in sign, thus cancelling the first order in φ contribution of the persistent current in the extended system (this was also the result in [18]). This is exactly what was obtained for the one-dimensional clean ring. To remind, the magnitude of both diamagnetic and paramagnetic terms in that calculation was $i_0\sqrt{\mu/\epsilon_0}$, which in one-dimensional case is precisely $i_0 N$. Then it is clear, that the disorder averaging in the extended system is nothing but a smoothing of the relevant quantity over the spectrum of the clean system, and since the spectra of the one-dimensional clean ring and our extended system defined by (2.7) with zero potential are similar (the reduced flux acting only along one axis), it is not surprising after all to obtain the same results.

All what has been said remains true for the third order term in φ of the persistent current. Averaging over the disorder is very much alike smoothing the third order contribution of the current in the clean one-dimensional ring. Indeed consider the expression for I_3 in terms of Green's functions, which can be derived by substituting the expansion (2.53) into (2.52),

$$\begin{aligned} I_3 &= -i_0\epsilon_0 \int_{-\infty}^{\infty} \frac{dE}{2\pi i} \mathrm{Tr}\, f(E) \left(G_0^A(E) G_0^A(E) - \text{c.c.} \right) \\ &\quad - \frac{2i_0\epsilon_0}{m} \int_{-\infty}^{\infty} \frac{dE}{\pi i} \mathrm{Tr}\, f(E) \left(G_0^A(E) p_x G_0^A(E) p_x G_0^A(E) - \text{c.c.} \right) \\ &\quad - \frac{i_0\epsilon_0}{m^2} \int_{-\infty}^{\infty} \frac{dE}{\pi i} \mathrm{Tr}\, f(E) \left(G_0^A(E) p_x G_0^A(E) p_x G_0^A(E) p_x G_0^A(E) p_x - \text{c.c.} \right). \end{aligned} \tag{2.57}$$

After the disorder averaged Green's functions (2.55) are inserted into (2.58), the integrals over the momenta $\mathbf{p}$ (the traces) can be performed, and each term which appears has the form of one of the terms in (2.16), except that the sum over discrete index l there should be substituted by an integral over the energies including the three-dimensional density of states. We then obtain

$$\begin{aligned} I_3 &= -i_0\epsilon_0 \int_{-\infty}^{\infty} dE\, f'(E)\rho(E) - \frac{4i_0\epsilon_0}{3} \int_{-\infty}^{\infty} dE\, f''(E)\rho(E)E \\ &\quad - \frac{4i_0\epsilon_0}{15} \int_{-\infty}^{\infty} dE\, f'''(E)\rho(E)E^2. \end{aligned} \tag{2.58}$$

In fact would we have used the one-dimensional density of states, and one-dimensional momenta to integrate (2.58), the result would have been exactly equivalent to the smoothing of the current in the one-dimensional ring. This once again makes the point that the so called disorder averaging is nothing but one among many other ways to smooth the physical quantities over the energies (another way

for instance is the use of the Euler-Maclaurin summation formula). The factors appearing in (2.58) because of the angle integration of the three-dimensional momenta combine with the three-dimensional density of states (one has to keep in mind that the three-dimensional density of states is proportional to the square root of the chemical potential, whereas in one-dimensional it is inversely proportional to $\sqrt{\mu}$) to give again a zero result for the smoothed I_3. This was not unexpected, as we said earlier, because of the similar nature of the spectrum in the one-dimensional and the three-dimensional systems.

Of course, we would like now to consider the real spectrum of the wide disordered ring and to calculate the smoothed persistent current to various orders of the perturbation theory in the flux. This is a very difficult problem for the following reasons: we have to know the exact distribution of the energy levels in our ring; even if we knew this distribution, it is highly probable that it would turn out to be a function so complex, that any formal manipulations needed to do the smoothing would be impossible to perform. Bearing this in mind, we would like in the rest of this section to present few arguments, that lack the rigor, therefore their validity is questionable. Nevertheless, in our opinion they do indicate the limitations of the currently accepted approaches as well as hopefully suggest the ways to progress.

First we would like to understand if vanishing of the smoothed first order in the perturbation series of the current is a general phenomenon, and not simply a mere coincidence that the smoothed I_1 came out to be zero in three different models. We return to the general expression (2.54) of I_1. It is clear that the first, diamagnetic term is always equal to $-i_0 N$. The second, paramagnetic term can be expressed in terms of the eigenstates of H_0, $|n\rangle$, having an energy E_n, in the following way (by writing out the trace explicitly and then performing the integral over E)

$$I_1^P = -\frac{i_0}{m} \sum_{n,m} \frac{f(E_n) - f(E_m)}{E_n - E_m} |(p_x)_{nm}|^2 , \tag{2.59}$$

here $(p_x)_{nm} = \langle n | p_x | m \rangle$ is the matrix element of the operator p_x; in the case where $n = m$ instead of the fraction in (2.59) one should take the derivative of the Fermi-Dirac distribution $f'(E_n)$. It is reasonable to think that the main contribution to (2.59) will come from the pairs of levels with almost the same energies. Those terms to a very good approximation involve the derivative $f'(E_n)$, which at $T = 0$ is proportional to the delta function $\delta(E_n - \mu)$. If now the paramagnetic term in (2.54) has a delta function as a factor in the integrand, it is justified to substitute $p_x^2/2m$, which also appears in the integrand, by $\mu/3$. Then, doing the integral over E , we obtain

$$I_1^P = -\frac{2 i_0 \mu}{3} \lim_{E_n \to E_m} \sum_{n,m} \frac{f(E_n) - f(E_m)}{E_n - E_m}. \tag{2.60}$$

The sum in (2.60) is the static density-density response function in the long wavelength limit for a non-interacting system [19]

$$\lim_{\mathbf{q} \to 0} \chi(\mathbf{q}, \omega = 0) = \lim_{E_n \to E_m} \sum_{n,m} \frac{f(E_n) - f(E_m)}{E_n - E_m}. \tag{2.61}$$

In the long wavelength limit the density-density response function is known to satisfy the compressibility sum rule, which can be derived from certain macroscopic arguments [19]

$$\lim_{\mathbf{q}\to 0}\chi(\mathbf{q},\omega=0)=-\left(\frac{\partial N}{\partial\mu}\right)_V. \tag{2.62}$$

The derivative of the particle number with respect to the chemical potential in (2.62) is equal to the inverse mean level spacing at the Fermi energy (this is true in the leading order of the weak disorder perturbation theory). Since, according to the Byers-Yang theorems the energy is an even function of φ, the correction due to the magnetic flux to the mean level spacing begins with the second order term and therefore is not relevant to the calculation of I_1^p. Hence

$$\left(\frac{\partial N}{\partial\mu}\right)_V = V\rho(\mu) \tag{2.63}$$

and substituting (2.62) into (2.61) and then into (2.60) we obtain that the paramagnetic term is equal to $i_0 N$, thus exactly cancelling the diamagnetic contribution. This argument is not rigorous, because it is unclear to what extent the ratio in (2.59) can be substituted by the derivative of the Fermi-Dirac distribution.

An interesting observation is appropriate here about the third order term of the persistent current I_3. Before starting the discussion, we would like to make few assumptions about the Hamiltonian H_0. First, assume that there are no degeneracies in the spectrum of H_0. This should hold reasonably well if the system is disordered. Second, the expectation value of the operator p_x in the eigenstate of H_0 equals to zero. This statement follows from the first assumption, if the Hamiltonian is invariant under time reversal. The third assumption is that the energy levels are sufficiently smooth functions of the reduced flux. Now consider the third term in (2.58), $I_3^{(3)}$, which contains the fourth power of the momentum. Performing the trace over the exact eigenstates of the Hamiltonian H_0, then integrating over the complex energy along the contour in the upper halfplane, the following exact expression is obtained (true under the above assumptions)

$$\begin{aligned} I_3^{(3)} &= -\frac{4i_0\epsilon_0}{m^2}\sum_n\left(f'(E_n)\left(\sum_m\frac{|(p_x)_{nm}|^2}{E_n-E_m}\right)^2-2f(E_n)\sum_{m,k}\frac{|(p_x)_{nm}|^2\,|(p_x)_{nk}|^2}{(E_n-E_m)^2(E_n-E_k)}\right) \\ &\quad -\frac{8i_0\epsilon_0}{m^2}\sum_n f(E_n)\sum_{m,k,l}\frac{(p_x)_{nm}(p_x)_{mk}(p_x)_{kl}(p_x)_{ln}}{(E_n-E_m)(E_n-E_k)(E_n-E_l)}, \end{aligned} \tag{2.64}$$

here n, m, k and l are indices labeling the eigenstates of H_0; the sums in (2.64) do not contain those combinations of indices, that make any of the denominators to vanish. Of course (2.64) can be checked doing the usual non-degenerate perturbation theory in φ for the energy levels of the total Hamiltonian H (recall our first assumption) and then substituting the resulting second and fourth order expressions into the formula for the total current - for instance into (2.45).

Perhaps somewhat unexpectedly formula (2.64) can be obtained from an integral over different combination of Green's functions than that in (2.58). Indeed making

use of our assumptions, one can convince him/herself that the following expression, when integrated over the complex energy along the contour in the upper halfplane, yields exactly (2.64)

$$I_3^{(3)} = -\frac{2i_0\epsilon_0}{m^2}\int_{-\infty}^{\infty}\frac{dE}{\pi i}\mathrm{Tr}f(E)\left(G_0^A(E)p_xG_0^A(E)p_xG_0^A(E)p_xG_0^R(E)p_x - \text{c.c.}\right). \quad (2.65)$$

A natural next step to do is to average this expression over the disorder, making use of the average Green's functions given in (2.55), and neglecting the correlations between different Green's functions due to disorder. This should give the leading contribution in weak disorder for $I_3^{(3)}$. Surprisingly enough, the result we obtain is not equal to $i_0\epsilon_0/\Delta$, the contribution of the third term in (2.58) (Δ is the mean level spacing at the Fermi level, equal to $1/V\rho(\mu)$). Instead, we find integrating (first over the energy (2.65) by parts, then the remaining integral over the momenta is easy) that

$$I_3^{(3)} = \frac{32\tau^2 i_0\epsilon_0\mu^2}{5\hbar^2\Delta}. \quad (2.66)$$

This is a much larger contribution than previously obtained $i_0\epsilon_0/\Delta$. In fact it is proportional to $E_C^2/\hbar\Delta$, where $E_C = \hbar D/R^2$ is the Thouless (correlation) energy (D is the diffusion constant). We end up here with a paradox. Two exact expressions (2.58) and (2.65), which are equal under very reasonable assumptions, lead us to two different results after the conventional disorder average is performed. We feel that the resolution of this paradox is necessary to achieve real progress on the problem of the average grand-canonical persistent currents. However the lesson which this discussion teaches us is that the third order in the flux of the smooth persistent current is apparently sensitive to the properties of the energy spectrum - the same conclusion as was reached studying one-dimensional models.

At last the following remark is in order. The thick disordered ring threaded by the solenoid can be modeled using Random Matrix Theory (RMT). The most suitable approach to describe the transition between the Gaussian Orthogonal Ensemble (GOE) and the Gaussian Unitary Ensemble (GUE), was obtained analytically by Pandey and Mehta [20], where the statistics of an $N \times N$ matrix Hamiltonian of the form

$$H = H(S) + i\alpha H(A), \quad (2.67)$$

was studied; here $H(S)$ is a real symmetric matrix, $H(A)$ is a real antisymmetric matrix, and α is a parameter, which interpolates between the two ensembles. The statistics of the levels of (2.67) was shown by Dupuis and Montambaux [21] to agree very well with that in a real metallic ring, turning on the magnetic flux in the solenoid. They also mapped the parameters of the RMT to the physical quantities, characterizing the spectrum of the metallic ring. Thus for instance the parameter α was shown to correspond to the reduced flux φ.

We could in principle find the smoothed persistent current within the RMT. For the first order in the reduced flux, we would start from

$$I_1 = -\frac{1}{h}\sum_n f(E_n)E_n'', \quad (2.68)$$

where the summation index n is over all the eigenvalues of the Hamiltonian (2.67). The most intuitive way to smooth this expression is to calculate its average in the RMT. It would be enough to smooth I_1 at zero temperature and then only the average curvature at $\varphi = 0$ is needed. However the exact curvature distribution function is not known for (2.67), the only available results are for the two by two $N = 2$ matrices [22]. In this case the distribution function of the curvature at a small reduced flux is symmetric, therefore the average vanishes. Again it means no first order persistent current. For the third order, the general expression is

$$I_3 = -\frac{1}{h}\sum_n \left(f(E_n)\frac{E_n^{\mathrm{iv}}}{6} + f'(E_n)\frac{(E_n'')^2}{2} \right). \tag{2.69}$$

To find the smoothed I_3 we need the second moment of the curvature and the average of the fourth derivative at $\varphi = 0$. Surprisingly enough, the second moment of the curvature was found [22] to diverge at zero reduced flux. However the distribution function for the fourth derivative was not calculated. Yet it would be important and interesting thing to do, checking if the singularity of the second moment of the curvature is not cancelled by the average of the fourth derivative.

2.5 The average canonical persistent current.

Up to now, we considered the grand-canonical persistent current, i.e. keeping the chemical potential fixed, independent of the flux. We would like now to study the behavior of the current in the canonical ensemble, when the total particle number is kept constant instead. We can preserve the constancy of the particle number by making the chemical potential flux dependent.

The definitions of the grand-canonical and canonical currents are respectively

$$I_{GC} = -\frac{1}{h}\sum_n f\left(E_n(\varphi),\mu\right)\frac{\partial E_n(\varphi)}{\partial\varphi}, \tag{2.70}$$

$$I_C = -\frac{1}{h}\sum_n f\left(E_n(\varphi),\mu(\varphi)\right)\frac{\partial E_n(\varphi)}{\partial\varphi}, \tag{2.71}$$

here the index n runs over the exact eigenstates of the Hamiltonian; the dependence of the Fermi-Dirac distribution on the chemical potential is displayed explicitly. We will look now for the difference between the persistent currents $I_{GC} - I_C$ in these two ensembles, expanded in powers of the reduced flux φ. The demonstration here will essentially follow the work of Altshuler, Gefen and Imry [23] (see also [24]).

We assume that the energy for all eigenstates is an even and sufficiently smooth function of φ, so that the expansion in the reduced flux for the n'th energy level begins with $E_n(\varphi) = E_n + E_n''\varphi^2/2$. At small flux the chemical potential changes by a small amount $\delta\mu(\varphi)$, and we now expand (2.71) in this small quantity. As a result we obtain to the lowest order in the expansion of $I_{GC} - I_C$

$$I_{GC} - I_C = -\frac{1}{h}\sum_n f'\left(E_n(\varphi),\mu\right)E_n''\delta\mu(\varphi)\varphi + o(\varphi^2). \tag{2.72}$$

The small $\delta\mu(\varphi)$ in its turn can be found from the requirement that in the canonical ensemble the total particle number should be independent of the reduced flux. Expanding thus the right-hand side of

$$N = \sum_n f\left(E_n(\varphi), \mu(\varphi)\right),$$

we find to lowest order (both the energy and the chemical potential are functions of φ)

$$\sum_n f'(E_n,\mu)E_n''\frac{\varphi^2}{2} - \sum_n f'(E_n,\mu)\delta\mu(\varphi) = 0. \tag{2.73}$$

The small variation of the chemical potential can be inferred from (2.73). We see that it is proportional to the second power of the reduced flux - in agreement with the Byers-Yang theorems. Inserting (2.73) into the expression for the current difference (2.72) finally yields

$$I_{GC} - I_C = -\frac{1}{2h}\frac{(\sum_n f'(E_n,\mu)E_n'')^2}{\sum_n f'(E_n,\mu)}\varphi^3. \tag{2.74}$$

The denominator of this expression is just minus the derivative of the particle number with the chemical potential, which is equal to the inverse mean level spacing at the Fermi energy, $1/\Delta$. However the sum $\sum_n f'(E_n,\mu)E_n''$ when smoothed over the spectrum vanishes as was shown by E. Akkermans in [25]. In the case of thick ring, its square does not vanish, because the disorder couples the two sums in a nontrivial way. In fact the non vanishing part of $(\sum_n f'(E_n,\mu)E_n'')^2$ can be shown to be proportional to the expression for the fluctuations of the conductance. This quantity was calculated in [26] and found to be constant of order of unity. Therefore the difference $I_{GC} - I_C$ is non-zero at the third and higher orders of the φ expansion; it is paramagnetic and of the order of Δ/h (small compared to the experimentally found value).

We summarize here the main results of this chapter. The smooth persistent current was found to vanish in the clean one-dimensional ring. Introducing one delta-like impurity (Kronig-Penney model) results in a finite smooth magnetic response. The smooth current is therefore sensitive to level repulsion in the spectrum. On the other hand the zero magnetic response was obtained in Scarf's model, which at zero flux has a non-degenerate spectrum. For three-dimensional (thick) ring the disorder average of the current is shown to be equivalent to the smoothing over the spectrum of a clean system. The possibility of the smoothing over the spectrum of a disordered system is discussed. Finally we find that the grand-canonical current is larger than its canonical counterpart by a quantity of magnitude Δ/h.

Chapter 3

The magnetic response in the Aharonov-Bohm problem.

3.1 General remarks.

Though in the previous chapter we set out to solve the Schrödinger equation characteristic to Aharonov-Bohm (A-B) setup, we never treated the equation (2.2) as it is written. Instead, we took up the Bloch problem, described by the equation (2.7). The vector potential entering this equation does not depend on **r**, being much simpler than the original A-B vector potential, which is inversely proportional to the distance from the magnetic coil. Now we consider the problem of the response to the A-B vector potential in its full generality, though neglecting the disorder. This should be compared with the problem of the magnetic response considered in the previous chapter - current in a two-dimensional cylinder with a magnetic solenoid threading it along its axis.

We recall the scattering problem considered by Aharonov and Bohm. We consider a free electron confined to the plane. The plane is pierced through its origin by an infinitely thin solenoid of magnetic flux Φ. The vector potential due to the solenoid (in the following we shall call it the Aharonov-Bohm (A-B) flux line) is given by the equation (2.1). The motion of an electron in this A-B potential is governed by the Schrödinger equation

$$-\frac{\hbar^2}{2m}\left(\frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial}{\partial r}\psi\right)+\frac{1}{r^2}\left(\frac{\partial}{\partial\theta}-i\varphi\right)^2\psi\right)=E\psi, \tag{3.1}$$

here the reduced flux is as previously $\varphi=\Phi/\Phi_0$. The question we are formulating is to find the total persistent current (all current due to the ideal solenoid is persistent, non-dissipative) and the magnetic moment at zero temperature of the electron gas due to the A-B flux line. There have been few related calculations in the recent years. The second virial coefficient for the free anyon gas has been found [27], connected to the total persistent current; M. V. Berry calculated the total charge pushed to infinity by the A-B flux line in the semi-classical limit [28]. The question as it is formulated here was posed for the first time at the Technion [29] (incidentally the work of Aharonov and Bohm was initiated there too) and solved using the scattering

theory. The subtle point of correctly regularizing the diverging expression for the total persistent current within the scattering approach was later discussed in [30].

We propose a different method to find the persistent current, which is flexible enough for the calculation of the magnetic moment. Our strategy will be to start from the quantum mechanical definition of the current density through the wave functions, and to perform the required sums and integrals.

First we need the wave functions that solve the Schrödinger equation (3.1). Denoting the conserved angular momentum by l, the general solution is

$$\psi(r,\theta) = \left(A_l J_{|l-\varphi|}(kr) + B_l J_{-|l-\varphi|}(kr)\right) e^{il\theta}, \tag{3.2}$$

here A_l and B_l are normalization constants, and we will assume $0 \leq \varphi < 1$. We will require that $B_l = 0$, because the particle density should not diverge at the origin of the coordinates, where the solenoid is located (Bessel functions with negative indices diverge for zero argument). This argument is not as innocuous as it seems. Strictly speaking the mode with the angular momentum $l = -1$ would not yield a diverging density. A deeper discussion of these issues would lead us to the theory of self-adjoint extensions of the Hamiltonian [31]. We will fix now the constant A_l by choosing the following normalization of the wave function

$$A_p^2 \int_{-\infty}^{\infty} \frac{d\mathbf{k}}{(2\pi)^2} J_p(kr)\, J_p(kr') = \frac{1}{2\pi r}\delta(r-r'), \tag{3.3}$$

here $E = \hbar^2 k^2/2m$; p is an arbitrary index. Using an identity

$$\int_0^{\infty} dk\, k J_p(kr)\, J_p(kr') = \frac{1}{r}\delta(r-r'),$$

we obtain $A_l^2 = 1$. We will check if this normalization in the case of free particles ($\varphi = 0$) gives the correct density of states. The Green's function can be expressed in terms of the wave functions (the normalization $A_l = 1$ is meant)

$$\begin{aligned} G(\mathbf{r},\mathbf{r},E) &= \int \frac{d\mathbf{k}}{(2\pi)^2} \sum_m J_m^2(kr) \frac{1}{E - \frac{\hbar^2 k^2}{2m}} \\ &= \frac{1}{2\pi} \int_0^{\infty} \frac{dk\, k}{E - \frac{\hbar^2 k^2}{2m}} = \frac{m}{\pi\hbar^2} \int_0^{\infty} \frac{dk\, k}{q^2 - k^2}. \end{aligned} \tag{3.4}$$

The density of states for the free particles is (using the definition of the density of states through the Green's function)

$$\begin{aligned} \rho(E) &= -\frac{1}{\pi}\mathrm{Im}\frac{S}{2\pi}\int_0^{\infty} \frac{dk\, k}{E + i\eta - \frac{\hbar^2 k^2}{2m}} \\ &= \lim_{\eta\to 0} \frac{S}{2\pi^2}\int_0^{\infty} dk\, k \frac{\eta}{\left(E - \frac{\hbar^2 k^2}{2m}\right)^2 + \eta^2} = \frac{S}{2\pi}\int_0^{\infty} dk\, k\delta\left(E - \frac{\hbar^2 k^2}{2m}\right) = \frac{Sm}{2\pi\hbar^2}, \end{aligned} \tag{3.5}$$

where S the area of the domain with the particles. We obtain the well-known result for the two-dimensional density of states, therefore our normalization is correct.

3.2 The persistent current.

Having determined the wave functions of the problem, we can use the quantum-mechanical definition of the current density of an ψ

$$\mathbf{j}(\mathbf{r}) = \frac{\hbar}{m}\mathrm{Im}\left(\psi^*(\nabla - \frac{ie}{\hbar c}\mathbf{A})\psi\right).$$

To find the total current density, one has to sum over all the occupied states (in our case the sum is over the angular momentum l, and the integral should be taken over the momentum k, which is a continuous variable). From symmetry considerations it is clear that the current density has the azimuthal direction

$$\begin{aligned} j_\theta &= \int_0^{k_F} \frac{d\mathbf{k}}{(2\pi)^2} \sum_{l=-\infty}^{\infty} \left(\frac{\hbar}{mr} l J^2_{|l-\varphi|}(kr) - \frac{1}{2\pi r}\frac{\Phi e}{mc} J^2_{|l-\varphi|}(kr) \right) \\ &= \int_0^{k_F} \frac{d\mathbf{k}}{(2\pi)^2} \sum_{l=-\infty}^{\infty} \frac{\hbar}{mr} (l-\varphi) J^2_{|l-\varphi|}(kr). \end{aligned} \tag{3.6}$$

For any finite kr the sum in Eq. (3.6) converges absolutely, due to the large l asymptotic behavior of the Bessel function [8]

$$J_l(kr) \sim \frac{1}{\sqrt{2\pi l}} \left(\frac{ekr}{2l}\right)^l \tag{3.7}$$

(we are grateful to J. Avron for this remark). The integral over the momentum k is taken up to the Fermi momentum - the largest occupied one, k_F. The total current is the radial integral of the total current density (3.6)

$$I = \int_0^R dr\, j_\theta = \int_0^R dr \int_0^{k_F} \frac{d\mathbf{k}}{(2\pi)^2} \sum_l \frac{\hbar}{mr} (l-\varphi) J^2_{|l-\varphi|}(kr). \tag{3.8}$$

We take here a disc of (large) radius R to be the domain where our system is defined. The radius of the disc will be later taken to infinity. In fact a large parameter in our problem is $k_F R \equiv \Lambda$. Basically in the following we shall look for an expansion of the total persistent current in powers of $1/\Lambda$.

We start therefore simplifying the expression in (3.8). To this end advantage is taken of the Lommel's formula. Since this identity is at the very base of our approach we feel that its derivation would be desirable here [32]. The following recurrence formulas are true for the Bessel functions

$$\begin{aligned} J_{p-1}(x) + J_{p+1}(x) &= \frac{2p}{x} J_p(x) \\ J_{p-1}(x) - J_{p+1}(x) &= 2\frac{dJ_p(x)}{dx}. \end{aligned} \tag{3.9}$$

Multiplying these two identities, we obtain

$$J^2_{p-1}(x) - J^2_{p+1}(x) = \frac{2p}{x}\frac{dJ^2_p(x)}{dx} \tag{3.10}$$

Consider now this formula substituting $p+2$ for p,

$$J_{p+1}^2(x) - J_{p+3}^2(x) = \frac{2(p+2)}{x}\frac{dJ_{p+2}^2(x)}{dx},$$

then $p+4$, etc. ad infinitum. Then sum up all these equations. The following identity will result

$$J_{p-1}^2(x) = \sum_{n=0}^{\infty}\frac{2}{x}(p+2n)\frac{dJ_{p+2n}^2(x)}{dx},$$

or, after an integration,

$$\sum_{n=0}^{\infty}\frac{2}{x}(p+2n)J_{p+2n}^2(x) = \frac{1}{2}\int_0^x tJ_{p-1}^2(t)\,dt. \tag{3.11}$$

We will apply now the Lommel's formula (3.11) for the sum entering the expression of the total persistent current (3.8)

$$\begin{aligned}
&\sum_{l=-\infty}^{\infty}(l-\varphi)\,J_{|l-\varphi|}^2(kr) = \sum_{l=1}^{\infty}(l-\varphi)\,J_{|l-\varphi|}^2(kr) - \sum_{l=0}^{\infty}(l+\varphi)\,J_{|l+\varphi|}^2(kr)\\
&= \sum_{n=0}^{\infty}(1-\varphi+2n)\,J_{1-\varphi+2n}^2(kr) + \sum_{n=0}^{\infty}(2-\varphi+2n)\,J_{2-\varphi+2n}^2(kr)\\
&- \sum_{n=0}^{\infty}(\varphi+2n)\,J_{\varphi+2n}^2(kr) - \sum_{n=0}^{\infty}(1+\varphi+2n)\,J_{1+\varphi+2n}^2(kr)\\
&= \frac{1}{2}\int_0^{kr} t\left(J_{-\varphi}^2(t) - J_{\varphi}^2(t) + J_{1-\varphi}^2(t) - J_{\varphi-1}^2(t)\right)dt
\end{aligned} \tag{3.12}$$

We succeeded hence to convert the difficult sum into a relatively simple integral. Inserting relationship (3.12) into (3.8), a closed formula for the total current follows

$$I = \frac{\hbar}{4\pi m}\int_0^R\frac{dr}{r}\int_0^{k_F}dk\,k\int_0^{kr}t\left(J_{-\varphi}^2(t) - J_{\varphi}^2(t) + J_{1-\varphi}^2(t) - J_{\varphi-1}^2(t)\right)dt. \tag{3.13}$$

The rest of this section is devoted to the evaluation of this expression (all four terms here have clearly the same structure).

We begin by transforming the general integral entering (3.13) (we denote it by I_p) by more or less elementary operations, involving no more than integration by parts. This leaves us with the two double integrals

$$\begin{aligned}
I_p &= \int_0^R\frac{dr}{r}\int_0^{k_F}dk\,k\int_0^{kr}tJ_p^2(t)\,dt = \int_0^R\frac{dr}{r^3}\int_0^{k_Fr}dy\,y\int_0^{y}tJ_p^2(t)\,dt\\
&= \int_0^R\frac{dr}{r^3}\left(\frac{y^2}{2}\int_0^{y}tJ_p^2(t)\,dt\Big|_0^{k_Fr} - \frac{1}{2}\int_0^{k_Fr}dy\,y^3J_p^2(y)\right)
\end{aligned}$$

$$= \int_0^R \frac{dr}{2r^3}\left((k_F r)^2 \int_0^{k_F r} t J_p^2(t)\,dt - \int_0^{k_F r} dy\, y^3 J_p^2(y)\right)$$

$$= \frac{k_F^2}{2}\int_0^{k_F R}\frac{dy}{y}\int_0^y t J_p^2(t)\,dt - \frac{k_F^2}{2}\int_0^{k_F R}\frac{dy}{y^3}\int_0^y t^3 J_p^2(t)\,dt. \qquad (3.14)$$

There are now two terms. We take the second one and transform it in the same spirit as previously

$$\frac{k_F^2}{4}\int_0^{k_F R} d\left(\frac{1}{y^2}\right)\int_0^y t^3 J_p^2(t)\,dt = \frac{k_F^2}{4}\left(\frac{1}{y^2}\int_0^y t^3 J_p^2(t)\,dt\Big|_0^{k_F R} - \int_0^{k_F R} t J_p^2(t)\,dt\right)$$

$$= \frac{1}{4R^2}\int_0^{k_F R} dt\, t^3 J_p^2(t) - \frac{k_F^2}{4}\int_0^{k_F R} t J_p^2(t)\,dt. \qquad (3.15)$$

Before going to the first term of (3.14), we quote few indefinite integrals over the powers of the Bessel function, which will be useful in the following (these identities can be checked by differentiating them)

$$\int^y t J_p^2(t)\,dt = \frac{y^2}{2}\left(J_p^2(y) + J_{p+1}^2(y) - \frac{2p}{y}J_p(y)\,J_{p+1}(y)\right), \qquad (3.16)$$

$$\int^y t^3 J_p^2(t)\,dt = \frac{y^4}{6}\left(J_p^2(y) + J_{p+1}^2(y)\right) - \frac{t^3}{3}(p-1)J_p(t)J_{p+1}(t) + \frac{2}{3}(p-1)\int^y t^2 J_p(t)J_{p+1}(t)dt, \qquad (3.17)$$

$$\int^y t^2 J_p(t)J_{p+1}(t)dt = \frac{y^2}{2}\left(pJ_p^2(y) + (p+1)J_{p+1}^2(y)\right) - p(p+1)y\,J_p(y)J_{p+1}(y), \qquad (3.18)$$

$$\int^y J_p(t)J_{p+1}(t)dt = p\int^y \frac{J_p^2(t)}{t}dt - \frac{J_p^2(y)}{2}. \qquad (3.19)$$

Returning now to the first term in (3.14), we integrate it using (3.16) and (3.19)

$$\frac{k_F^2}{2}\int_0^{k_F R}\frac{dy}{y}\int_0^y t J_p^2(t)\,dt = \frac{k_F^2}{4}\int_0^{k_F R} dy\, y\left(J_p^2(y) + J_{p+1}^2(y)\right) - \frac{k_F^2}{4}p^2\int_0^{k_F R}\frac{J_p^2(y)}{y}dy + \frac{k_F^2}{8}pJ_p^2(y)\Big|_0^{k_F R} \qquad (3.20)$$

Substituting the two terms (3.20) and (3.15) into the expression for the general integral I_p (3.14), we obtain

$$I_p = \frac{1}{4R^2}\int_0^{k_F R} dt\, t^3 J_p^2(t) + \frac{k_F^2}{4}\int_0^{k_F R} t J_{p+1}^2(t)\,dt - \frac{k_F^2}{4}p^2\int_0^{k_F R}\frac{J_p^2(y)}{y}dy + \frac{k_F^2}{8}pJ_p^2(y)\Big|_0^{k_F R} \qquad (3.21)$$

Using three identities (3.16), (3.17) and (3.19), I_p can be expressed entirely in terms of products of Bessel functions and powers, evaluated at $\Lambda = k_F R$ and 0, and one integral, whose asymptotic behavior as $\Lambda \to \infty$ is

$$\int_0^\Lambda \frac{J_p^2(y)}{y} dy \sim \frac{1}{2p} + O(\frac{1}{\Lambda}). \tag{3.22}$$

As a last step of this calculation we should find the asymptotic expansion of I_p, when as already mentioned, Λ is the large parameter. It is not difficult to do in principle, because we need only the well-known asymptotic expansion of the Bessel function for large arguments [32]. However in practice it is a messy calculation, because to be consistent, the leading term in the Bessel function expansion is insufficient, one has to take into account also the sub-leading term. Introducing the notation $\chi_p = \Lambda - (p/2 + 1/4)\pi$ and using the asymptotics of the Bessel functions, we obtain

$$\begin{aligned}
4R^2 I_p \sim & \frac{\Lambda^3}{3\pi}\left(1 - 2\frac{4p^2-1}{8\Lambda}\cos\chi_p \sin\chi_p - 2\frac{4(p+1)^2-1}{8\Lambda}\cos\chi_{p+1}\sin\chi_{p+1}\right) \\
& + \frac{\Lambda^3}{\pi}\left(1 - 2\frac{p+1}{\Lambda}\cos\chi_{p+1}\cos\chi_{p+2} - 2\frac{4(p+1)^2-1}{8\Lambda}\cos\chi_{p+1}\sin\chi_{p+1}\right) \\
& - \frac{p^2\Lambda^2}{2p} - \frac{\Lambda^3}{\pi}\left(\frac{4(p+2)^2-1}{4\Lambda}\cos\chi_{p+2}\sin\chi_{p+2}\right) \\
& - \frac{2\Lambda^3}{3\pi}(p-1)\cos\chi_p\cos\chi_{p+1} = -\frac{p}{2}\Lambda^2 + O(\Lambda).
\end{aligned} \tag{3.23}$$

The asymptotic expansion of I_p contains terms, which behave as Λ^3. However we have to go to the next order, Λ^2, because all leading order terms cancel out. The result in (3.23) has to be understood in the sense of the leading asymptotic behavior of I_p.

Finally, the total persistent current can be reconstructed from the integral I_p, since according to (3.13)

$$I = \frac{\hbar}{4\pi m}(I_{-\varphi} - I_\varphi + I_{1-\varphi} - I_{\varphi-1}). \tag{3.24}$$

Using the asymptotic result (3.23), the total persistent current is found to behave as

$$I \sim \frac{\hbar k_F^2}{8\pi m}(\varphi - \frac{1}{2}), \qquad 0 \le \varphi < 1. \tag{3.25}$$

To determine the persistent current for all values of the reduced flux, we recall that I is a periodic function of the reduced flux φ. As a result, the functional dependence of the persistent current on φ is singular - I is discontinuous at integer φ's. Our result disagrees with the conclusions in [29]. The discrepancy was shown in [30] to arise from the different regularizations of diverging sums. The expression (3.25) coincides with the result of the regularization by means of the zeta function. We would like to stress again that contrary to [30], we interpret (3.25) in an asymptotic sense. Namely it is the leading term in the large Λ asymptotic expansion of the total persistent current.

3.3 The magnetic moment.

The magnetic moment of the electron gas due to the A-B flux line can be calculated essentially repeating the scheme used to find the leading term in the asymptotic expansion of the total persistent current. The magnetic moment of the circular area (disc) of radius R is found by using the Biot-Savart law:

$$M = \frac{1}{2c}\int_S ds\, \mathbf{j}(\mathbf{r}) \times \mathbf{r} = \frac{\pi}{c}\int_0^R dr r j_\theta(r) r$$

$$= \frac{e\hbar}{2mc}\int_0^R dr r \int_0^{k_F} dk k \sum_{l=-\infty}^{\infty} (l+\varphi) J^2_{|l+\varphi|}(kr). \tag{3.26}$$

The sum in (3.26) was already calculated in the previous section. Substituting the identity (3.12) into the formula for the magnetic moment, we find an expression, reminiscent of the persistent current (3.13)

$$M = \frac{e\hbar}{2mc}\int_0^R dr r \int_0^{k_F} dk k \int_0^{k_F} dk\, k \int_0^{kr} t\left(J^2_{-\varphi}(t) - J^2_{\varphi}(t) + J^2_{1-\varphi}(t) - J^2_{\varphi-1}(t)\right) dt. \tag{3.27}$$

We would have now to integrate the integral M_p of the form

$$M_p = \int_0^R dr r \int_0^{k_F} dk k \int_0^{kr} dk\, k \int_0^{kr} t J^2_p(t)\, dt. \tag{3.28}$$

After an integration by parts, M_p is transformed into two double integrals

$$\begin{aligned} M_p &= \int_0^R \frac{dr}{r}\int_0^{k_F r} dy\, y \int_0^y t J^2_p(t)\, dt \\ &= \int_0^R \frac{dr}{r}\left(\frac{y^2}{2}\int_0^y t J^2_p(t)\, dt\Big|_0^{k_F r} - \frac{1}{2}\int_0^{k_F r} dy\, y^3 J^2_p(y)\right) \\ &= \frac{1}{2}\int_0^{k_F R} dy\, y \int_0^y t J^2_p(t)\, dt - \frac{1}{2}\int_0^{k_F R}\frac{dy}{y}\int_0^y t^3 J^2_p(t)\, dt. \end{aligned} \tag{3.29}$$

The first term in (3.29) can be transformed further

$$\frac{1}{2}\int_0^{k_F R} dy\, y \int_0^y t J^2_p(t)\, dt = \frac{1}{4}\left(y^2 \int_0^y t J^2_p(t)\, dt\Big|_0^{k_F R} - \int_0^{k_F R} t^3 J^2_p(t)\, dt\right). \tag{3.30}$$

The second term can be integrated using formulas (3.17) and (3.18)

$$-\frac{1}{2}\int_0^{k_F R}\frac{dy}{y}\int_0^y t^3 J^2_p(t)\, dt = -\frac{1}{2}\int_0^{k_F R} dt \frac{t^3}{6}\left(J^2_p(t) + J^2_{p+1}(t)\right)$$

$$\frac{1}{2}\int_0^{k_F R} dt\left(\frac{t^2}{3}(p-1)J_p(t)J_{p+1}(t)-\frac{t}{3}(p-1)\left(pJ_p^2(t)+(p+1)J_{p+1}^2(t)\right)\right)$$
$$+\frac{1}{2}\int_0^{k_F R} dt\,\frac{2}{3}p(p^2-1)J_p(t)J_{p+1}(t). \qquad (3.31)$$

Lastly the remaining integrals in (3.30) and (3.31) can be performed using all quoted integrals (3.16), (3.17), (3.18) and (3.19). The asymptotic formula (3.22) is used and everything is substituted into the expression for M_p.

Again considering Λ as the large parameter, we look for the asymptotic expansion of the integral M_p. The expansion of the Bessel function for the large argument is useful. With the same notations as in the previous section, we expand the two terms of (3.29)

$$M_p \sim \frac{\Lambda^3}{4\pi}\left(-\frac{4p^2-1}{4\Lambda}\cos\chi_p\sin\chi_p-\frac{4(p+1)^2-1}{4\Lambda}\cos\chi_{p+1}\sin\chi_{p+1}\right)$$
$$-\frac{\Lambda^2}{12\pi}(\cos\chi_p\sin\chi_p+\cos\chi_{p+1}\sin\chi_{p+1})+\frac{\Lambda^3}{4\pi}\left(1-\frac{p}{2\Lambda}\cos\chi_p\cos\chi_{p+1}\right)$$
$$-\frac{\Lambda^2(2p+1)}{12\pi}\cos\chi_p\sin\chi_p-\frac{\Lambda^3}{6\pi}(p-1)\cos\chi_p\sin\chi_p=0+\mathrm{O}(\Lambda). \qquad (3.32)$$

Therefore the leading order term (proportional to Λ^3) and the sub-leading one (proportional to Λ^2) in the asymptotic expansion of the magnetic momentum are zero. It would be desirable to continue this expansion to lower powers of Λ until a non-zero result is obtained. However the calculation becomes more and more time consuming.

We return to the question asked at the beginning of this chapter about the difference of the magnetic responses to a genuine A-B flux line and to a r-independent vector potential. To this end, the main result of this chapter, the leading asymptotic term of the persistent current, should be compared with the persistent current in a hollow cylinder threaded by the flux line. In the latter case, as was shown in the previous chapter, the smoothed persistent current (with which as we believe (3.25) should be compared) vanishes. In the former case, the persistent current is non-zero and furthermore has a non-trivial unexpected φ dependence.

Chapter 4

Random walk description of quantum localization.

In this chapter we investigate the problem of quantum localization of a particle in a random potential. This is a huge subject in its own (for a review see [33, 34]), of which we will touch only one aspect. We shall be motivated in our discussion by a model of random walk, which mimics the motion in a random potential. The asymptotic large time properties of the random walk turn out to be useful to justify this model. For instance the mean time spent by the random walker at a given site can be shown to be equivalent in the asymptotic limit to the heat kernel of the diffusion equation, a quantity to which we will return later.

As a paradigm of the problem of quantum localization it is worth to have in mind the Anderson model [35] given by

$$H = \sum_i V_i \, c_i^\dagger c_i + \sum_{ij} W_{ij} \, c_i^\dagger c_j, \tag{4.1}$$

where $W_{ij} = W$ for nearest neighbors i, j, and V_i is chosen randomly from the interval $[-V/2, V/2]$. For V/W larger than some critical value, Anderson proposed that all states are localized (in three dimensions), below this value there is a mobility edge and all states are extended. On the localized side of the mobility edge the insulating regime is entered, where the conductance g decays exponentially with the length of the system L. This decay is governed by the localization length ξ

$$g \propto e^{-\frac{L}{\xi}}. \tag{4.2}$$

When the mobility edge is approached from the localized side, the localization length diverges with a critical exponent ν [36].

Variety of techniques have been developed to determine ν, ranging from numerical finite size scaling [37], perturbation expansion in weak disorder [38], to field-theoretical calculations [39]. Among them one approach to find the critical exponent of the localization length is the self-consistent diagrammatic method developed by Vollhardt and Wölfle [40], see also [41]. The starting point is the perturbation expansion of the disorder average of the conductivity $\langle \sigma \rangle$ in the limit of a weak random potential ($1/k_F l$ is the small parameter, where k_F is the Fermi wavevector,

l the elastic mean free path). The perturbation theory for the Green's functions is formulated in the language of Feynman diagrams. The average conductivity is related to the Green's functions through the Kubo-Greenwood formula (E_F is the Fermi energy)

$$\langle\sigma(\omega)\rangle = \frac{e^2\hbar^3 L^3}{2\pi m^2}\int \frac{d\mathbf{k}_1}{(2\pi)^3}\frac{d\mathbf{k}_2}{(2\pi)^3}k_{1x}k_{2x}\langle G^R(\mathbf{k}_1,\mathbf{k}_2,E_F)G^A(\mathbf{k}_2,\mathbf{k}_1,E_F+\omega)\rangle. \quad (4.3)$$

The Green's operators are defined in (2.51). Replacing in a first approximation the disorder average of the product of two Green's functions by the product of the average Green's functions, the classical Drude formula is obtained

$$\langle\sigma_0(\omega)\rangle = \frac{ne^2\tau}{m(1-i\omega\tau)}, \quad (4.4)$$

where $\tau = l/v_F$, and n is the particle density. The first-order correction of the expansion in powers of $1/k_F l$ can be obtained by considering a summable class of irreducible diagrams, namely the maximally crossed diagrams. It is the weak localization correction to $\langle\sigma_0\rangle$

$$\langle\sigma(\omega)\rangle = \langle\sigma_0\rangle - \frac{e^2}{\pi\hbar}\int \frac{d\mathbf{q}}{(2\pi)^3}\frac{1}{q^2 - i\omega/D}. \quad (4.5)$$

The weak localization correction to the diffusion coefficient $D(\omega)$ can be derived from (4.5) using the relation $\sigma(\omega)/\sigma_0 = D(\omega)/D_0$, which follows from the hydrodynamic form of the density response function in the limit of long wavelength and low frequency [40, 41] (it can also be obtained from Einstein relation). Then in d dimensions we obtain

$$\frac{D(\omega)}{D_0} = 1 - \lambda d k_F^{2-d}\int_0^{k_0} dk \frac{k^{d-1}}{(-i\omega/D_0) + k^2}. \quad (4.6)$$

Here k_0 is a momentum cutoff of the order of the inverse mean free path, and λ is the weak scattering coupling constant $\lambda = \hbar/2\pi E_F\tau$. The self-consistent equation of Vollhardt and Wölfle is obtained by replacing in the right-hand side of (4.6) D_0 by $D(\omega)$. The diffusion coefficient is assumed to be momentum independent in order for the integrand in (4.6) to preserve the structure of the Green's function of the ordinary diffusion equation. Assuming the momentum dependence of the diffusion coefficient would lead us to consider anomalous diffusion [42].

On the localized side of the mobility edge, the static diffusion coefficient is zero, $\lim_{\omega\to 0}(-i\omega/D(\omega)) = \xi^{-2}$, and the self-consistent equation in this limit reduces to the transcendental equation for ξ,

$$1 = d\lambda(k_F\xi)^{2-d}\int_0^{k_0\xi} dy \frac{y^{d-1}}{1+y^2}. \quad (4.7)$$

The critical exponent ν can be found from this equation. We will illustrate how the method works for dimensions $2 < d < 4$ [40]. The right hand side of (4.7) is expanded in the inverse of the parameter $k_0\xi$, which is very large in the immediate vicinity of the mobility edge

$$1 = d\lambda\,(k_F\xi)^{2-d}\left(\frac{(k_0\xi)^{d-2}}{d-2} - \int_0^\infty dy \frac{y^{d-3}}{1+y^2} + \mathrm{O}((k_0\xi)^{d-4})\right). \tag{4.8}$$

Retaining only two explicitly written terms in the expansion, we obtain that the localization length diverges for $2 < d < 4$ as

$$\xi = k_F^{-1}\left(\frac{d-2}{d\lambda}\frac{1}{\Gamma(d/2)\Gamma(2-d/2)}\left|1-\frac{\lambda}{\lambda_c}\right|\right)^{-1/(d-2)}, \tag{4.9}$$

where

$$\lambda_c = \frac{d-2}{d}\left(\frac{k_0}{k_F}\right)^{2-d}. \tag{4.10}$$

The localization length ξ diverges with the critical exponent $\nu = 1/(d-2)$.

On the other hand the same critical exponents can be obtained using a heuristic argument due to Allen [43] based on a random walk model of the quantum localization. We review here Allen's criterion to determine when the localization of a quantum particle occurs. The particle is assumed to be a random walker in a d dimensional cubic lattice. It hops with a rate $W/2\hbar$, in time t making thus $n(t) = Wt/2\hbar$ steps. Lattice sites are labeled by energies ϵ_i which are distributed randomly with a uniform probability density of width V. During the time t the random walker visits $S(n)$ *distinct* sites, therefore the mean level spacing could be estimated as being approximately equal to $V/S(n)$. The random walk terminates and the particle gets localized when the individual energy levels can be resolved, that is when

$$\frac{V}{S(n)}t = \hbar. \tag{4.11}$$

Before stopping the particle moves diffusively, therefore asymptotically $n = \xi^2/a^2$, a is the lattice constant. Substituting the number of hops for the time in (4.11), we obtain

$$S(n) = u\,n, \tag{4.12}$$

here $u = 2V/W$ is a disorder dependent parameter. Making use of the first terms in the asymptotic expansion of $S(n)$ for large n for d dimensional lattice, (4.12) gives the critical behavior of the localization length ξ, which as was already mentioned, coincides with that derived from the self-consistent equation of Vollhardt and Wölfle (4.7). The formal similarity of these two approaches seems to indicate that a connection exists between them. Our purpose here is to demonstrate explicitly this connection, starting with Allen's equation (4.12) and deriving (4.7) from it.

In other words, we will provide a link between the heuristic argument due to Allen to determine the critical exponent of the localization length and the self-consistent diagrammatic method of Vollhardt and Wölfle describing the vicinity of

the Anderson metal-insulator transition. This work therefore on one hand side gives a rigorous justification of Allen's model, on the other hand it helps to appreciate the intuitive content of the self-consistent theory using the random walk analogy.

With this in mind, we return to the random walk description of the localization, concentrating on $S(n)$ - the mean number of distinct sites visited in a n step random walk. Consider the generating function, defined by

$$S(z) = \sum_{n=0}^{\infty} z^n S(n) \qquad (|z| \leq 1). \tag{4.13}$$

In terms of the generating function, equation (4.12) transforms to

$$S(z) = u \frac{z}{(1-z)^2}, \tag{4.14}$$

where the identity $\sum_{n=0}^{\infty} z^n n = z/(1-z)^2$ was used. It is still more convenient to use the generating function for the probabilities

$$G(\mathbf{x}_1 - \mathbf{x}_0, z) = z \sum_{n=0}^{\infty} z^n P(\mathbf{x}_1, \mathbf{x}_0; n), \tag{4.15}$$

$P(\mathbf{x}_1, \mathbf{x}_0; n)$ being the conditional probability for the walker to be at the site $\mathbf{x}_1$ after n hops, knowing that it started at $\mathbf{x}_0$. When $z = 1$, this generating function measures the mean time spent at the site $\mathbf{x}_1$. When $|z| \leq 1$, the sum in (4.15) always converges and has an integral representation [44]

$$G(\mathbf{x}_1 - \mathbf{x}_0, z) = a^d \int_{-\pi/a}^{\pi/a} \frac{d^d\mathbf{k}}{(2\pi)^d} \frac{e^{i\mathbf{k}(\mathbf{x}_1 - \mathbf{x}_0)}}{z^{-1} - \frac{1}{d}\sum_\mu \cos a k_\mu}, \tag{4.16}$$

here k_μ are the Cartesian coordinates of the vector $\mathbf{k}$. The generating functions $S(z)$ and $G(\mathbf{0}, z)$ can be shown to be connected through the following relation [44]:

$$S(z) = \frac{z}{(1-z)^2 G(\mathbf{0}, z)}. \tag{4.17}$$

Now inserting equation (4.17) into (4.14), we obtain

$$G(\mathbf{0}, z) = \frac{1}{u}. \tag{4.18}$$

This equation is a discrete Laplace transform of the main Allen's criterion (4.12) and as such should contain the same information. As we already mentioned, near the mobility edge (4.12) has to be understood as an asymptotic relation, valid in the large n limit. The corresponding limit for the equation (4.18) is provided by a Tauberian theorem for power series [45]. Its importance in our discussion seems to justify a short reminder, where we will follow the reference [45].

Tauberian theorem: Let $f(z)$ be a power series in z, z being a real variable, defined by

$$f(z) = \sum_{n=0}^{\infty} f_n z^n$$

and let the f_n be strictly positive. Suppose that in the limit $z \to 1$ the behavior of $f(z)$ is singular in the sense that

$$f(z) \sim (1-z)^{-\alpha} L\left(\frac{1}{1-z}\right)$$

where $L(x)$ is a slowly varying function and $\beta(x) = x^{\alpha} L(x)$ is a positive, monotonically increasing function of x for sufficiently large x. Then, in the limit $n \to \infty$, the partial sums of the f_n are approximated by

$$\sum_{j=0}^{n} f_j \sim \frac{\beta(n)}{\Gamma(1+\alpha)} = \frac{n^{\alpha} L(n)}{\Gamma(1+\alpha)}.$$

If moreover f_n is a monotonic function of n, at least from some value of N onwards, then

$$f_n \sim \frac{\beta'(n)}{\Gamma(1+\alpha)} = \frac{\alpha n^{\alpha-1} L(n) + n^{\alpha} L'(n)}{\Gamma(1+\alpha)}.$$

A function $L(x)$ is slowly varying at $x = \infty$, if, for every constant $c > 0$, it satisfies the condition

$$\lim_{x \to \infty} \frac{L(cx)}{L(x)} = 1.$$

We will go on applying this theorem to study the asymptotic limits of random walk. Suppose that the leading term of the characteristic function for the probabilities $G(\mathbf{0}, z)$ in the limit $z \to 1$ is of the form (this in fact is true in all dimensions d [44])

$$G(\mathbf{0}, z) \sim (1-z)^{\alpha-2} L^{-1}\left(\frac{1}{1-z}\right). \tag{4.19}$$

Then the leading asymptotic behavior of $S(z)$ is

$$S(z) \sim (1-z)^{-\alpha} L\left(\frac{1}{1-z}\right), \tag{4.20}$$

because $S(z)$ is related to $G(\mathbf{0}, z)$ through (4.17). The mean number of distinct sites visited in n steps $S(n)$ is a function that fulfills the restrictions needed in order to apply the Tauberian theorem, that is, it is positive monotonic function of n. Therefore in the limit $n \to \infty$, $S(n)$ is approximated by

$$S(n) \sim \frac{n^{\alpha-1} L(n)}{\Gamma(\alpha)}. \tag{4.21}$$

Near the mobility edge the localization criterion (4.12) should be thought of in an asymptotic sense. In the limit $n \to \infty$ it assumes the following form

$$\frac{n^{\alpha-2} L(n)}{\Gamma(\alpha)} = u. \tag{4.22}$$

The corresponding limit for the equation (4.18) is, according to (4.19),

$$(1-z)^{-\alpha+2} L\left(\frac{1}{1-z}\right) = u, \tag{4.23}$$

here $z \to 1$. This equation coincides with (4.22) after n is substituted by $1/(1-z)$ and the disorder dependent parameter u is redefined. Consequently, the solution of the equation (4.18) in its asymptotic limit, would lead to the same critical behavior of the localization length as that found by Allen, taking z equal to $1 - a^2/\xi^2$.

The last part of our demonstration is then to show that equation (4.18) with $z = 1 - a^2/\xi^2$ and $a/\xi \ll 1$, is equivalent to the self-consistent equation (4.7) under a similar condition $l/\xi \ll 1$, where l is the mean free path of the electron. It is helpful to bring these two together here in the form, indicating how close they are. First we rewrite the discrete Laplace transform of Allen's criterion, using the integral representation of the generating function $G(\mathbf{0}, z = 1 - a^2/\xi^2)$, given in (4.16),

$$a^d \int_{-\pi/a}^{\pi/a} \frac{d^d\mathbf{k}}{(2\pi)^d} \frac{1}{1 + \frac{a^2}{\xi^2} - \frac{1}{d}\sum_\mu \cos ak_\mu} = \frac{1}{u}, \tag{4.24}$$

where z^{-1} was expanded in the small parameter a/ξ. The equation of Vollhardt and Wölfle in its turn can be written as a similar expression

$$dk_F^{2-d} \int_0^{k_0} dk \frac{k^{d-1}}{\xi^{-2} + k^2} = \frac{1}{\lambda}. \tag{4.25}$$

A connection between these two equations should come as no surprise, because (4.25) is the diffusion limit of (4.24), which holds for the random walker on a discrete lattice. The diffusion approximation yields results basically equivalent to those obtained in the limit of large number of hops [46]. This diffusion approximation of the generating function $G(\mathbf{0}, z = 1 - a^2/\xi^2)$ is most easily derived in the limit $a \to 0$:

$$\lim_{a\to 0} \frac{1}{2da^{d-2}} G\left(\mathbf{0}, z = 1 - a^2/\xi^2\right) = \int_{-\infty}^{\infty} \frac{d^d\mathbf{k}}{(2\pi)^d} \frac{1}{\frac{2d}{\xi^2} + \mathbf{k}^2}. \tag{4.26}$$

Substituting (4.26) to (4.24), we obtain finally

$$S_d d \left(\frac{1}{a}\right)^{2-d} \int_0^{\infty} dk \frac{k^{d-1}}{\frac{2d}{\xi^2} + k^2} = \frac{1}{2u}, \tag{4.27}$$

here $S_d = 2\pi^{d/2}/\Gamma(d/2)$ is the area of the unit sphere in d-dimensional space. The upper integration limit should be taken equal to the finite cutoff when the integral diverges. Clearly, up to some minor modifications, equation (4.27) is identical to the self-consistent equation. The difference is in the smallest scale used to regularize the integral: whereas in Allen's approach it is the small, but finite lattice constant, there are two small lengths in the diagrammatic self-consistent theory - the mean free path and the inverse Fermi wave number.

We would like now to illustrate how the diffusion approximation leads to the asymptotic expression of the generating function, given for example in [44] and usually derived within the saddle point approximation [45]. Returning to (4.26), we transform its right-hand side, performing exactly the resulting integral (assuming that $2 < d < 4$ all integrals converge)

$$\int_{-\infty}^{\infty} \frac{d^d\mathbf{k}}{(2\pi)^d} \frac{1}{\kappa^2 + \mathbf{k}^2} = \int_{-\infty}^{\infty} \frac{d^d\mathbf{k}}{(2\pi)^d} \frac{1}{\mathbf{k}^2} - \int_{-\infty}^{\infty} \frac{d^d\mathbf{k}}{(2\pi)^d} \frac{\kappa^2}{(\kappa^2 + \mathbf{k}^2)\,\mathbf{k}^2} =$$

$$\int_{-\infty}^{\infty} \frac{d^d\mathbf{k}}{(2\pi)^d} \frac{1}{\mathbf{k}^2} - \frac{S^d}{(2\pi)^d} \kappa^{d-2} \int_0^{\infty} dy \frac{y^{d-3}}{1+y^2} =$$

$$\int_{-\infty}^{\infty} \frac{d^d\mathbf{k}}{(2\pi)^d} \frac{1}{\mathbf{k}^2} + \kappa^{d-2} \left(\frac{d}{2\pi}\right)^{d/2} \frac{\Gamma(1-d/2)}{2d},$$

here $\kappa = 2d/\xi^2$. This indeed coincides with [44].

Allen's approach is seen then to be closely related to the heuristic picture of the weak localization phenomenon. The transport of an electron in a disordered conductor is assumed to be diffusive. The diffusion coefficient is reduced from its classical value by a quantum correction, proportional to the probability of self-intersection of the diffusion path [47] (the so-called "return probability", related to the asymptotic limit of the heat kernel). Having now diffusion on a discrete lattice, it is not unreasonable to consider the diffusion path to be localized when the number of self-intersections is as large as the number of hops in the large time limit. However the number of self-intersections for the random walk can be estimated to be the difference of the number of steps and the number of distinct visited sites. Therefore this localization criterion is basically equivalent to Allen's one.

To conclude, we established that the criterion of Allen (4.12) and the self-consistent equation of Vollhardt and Wölfle (4.7) are related through Laplace transform. As a remark we mention that the same equation determines the critical behavior of the correlation length in the large n limit of the classical n-component vector Heisenberg model with an orthogonal $O(n)$ symmetry group. This relationship has to be further investigated, in particular it might give rise to the universal conductance fluctuations.

Another direction to extend this work is to consider the quantum localization problem when a (not necessarily uniform) magnetic field is applied to the system. In this case the Green's function (4.26), entering the localization criterion (4.7) (or equivalently (4.27)), no longer satisfies a simple diffusion equation. Instead the vector potential should be included in this equation by a usual minimal coupling scheme (this is only true in the semi-classical approximation, when the cyclotron radius exceeds the Fermi wavelength [48, 49]).

Chapter 5

Semi-classical spectrum of integrable systems in a uniform magnetic field.

5.1 Introduction.

With this chapter we begin the study of the response of finite-size quantum systems to a uniform magnetic field. With high fields in mind, we present here a semi-classical approach to calculate the energy spectrum of non-interacting electrons constrained to a finite two-dimensional domain and submitted to a uniform magnetic field (magnetic billiard). We limit ourselves to the integrable cases (i.e. systems, which in addition to the energy have another constant of motion). In the limit of high magnetic fields, determined by the inequality $\Phi \gg \Phi_0$ (here Φ is the total magnetic flux through the system and $\Phi_0 \equiv \frac{hc}{e}$ is the normal flux quantum), we are in the so called Integer Quantum Hall effect regime (IQHE) where the edge states associated with the boundary play a prominent role [50]. It is therefore important to have the spectrum of the magnetic billiard to a sufficient precision. Moreover the semi-classical methods allow us to appreciate more deeply the peculiarities of the spectra in presence of the magnetic field. Here we shall concentrate on the problem of non-interacting electrons in a semi-infinite plane, later presenting the results for the disc.

The classical dynamics of a magnetic billiard, allows for a natural separation between bulk and edge states which we are using in order to calculate the semi-classical spectrum. A first, least exact approximation is based on the Einstein-Brillouin-Keller quantization, which preserves this classical bulk-edge distinction by giving different quantization rules for each of them. This approximation is further improved by constructing the asymptotically matched WKB function and then finding its zeros corresponding to the energy levels. This matching of the different parts of the wave-function smoothes out the singularity between bulk and edge energies, resulting in a very good approximation for the exact spectrum. Finally we shortly discuss the method to calculate the spectrum of a disc in a magnetic field.

5.2 The classical dynamics

We consider a particle of positive charge e and mass m constrained to move in the semi-infinite plane. A uniform magnetic field B is applied perpendicular to the plane. Cartesian coordinates are defined such that the x axis is perpendicular to the boundary and the motion is confined to positive values of x. It is convenient to consider the boundary having a finite length L and therefore we impose periodic boundary conditions in the y direction ending with a semi-infinite cylinder geometry (fig.5.1).

In the Landau gauge $\mathbf{A} = (0, Bx)$, the Hamiltonian of the particle is

$$\mathcal{H} = \frac{1}{2m}\left({p_x}^2 + (p_y - \frac{e}{c}Bx)^2\right) \tag{5.1}$$

and the momentum is $\mathbf{p} = (m\dot{x}, m\dot{y} + \frac{e}{c}Bx)$. The total energy E and the y component p_y of the momentum are constants of motion, therefore the problem is integrable. In the four-dimensional phase space of the Cartesian coordinates and the corresponding momenta, each family of classical trajectories are winding on an invariant torus, defined by the two constants of motion.

The ensemble of trajectories splits naturally into two families: those that do not touch the boundary (bulk states) and others (edge states). Particles with the energy $E = mv^2/2$ (velocity $\mathbf{v} = (m\dot{x}, m\dot{y})$) go clockwise in circles of radius $r_c = \frac{v}{\omega}$, where $\omega = \frac{eB}{mc}$ is the cyclotron frequency. If the center of the orbit gets closer than r_c to the edge, the particle undergoes specular reflections and the cyclotron orbit center begins drifting along the edge (fig. 5.1). These are edge trajectories. The constant of motion p_y distinguishes between the edge and the bulk states: $p_y \geq p$ for the bulk trajectories, $p_y < p$ for the edge.

5.3 The EBK quantization.

We consider now the quantum-mechanical version of the same problem. Dirichlet boundary conditions are imposed on the wave function:

$$\psi(0, y) = 0. \tag{5.2}$$

This, together with the Schrödinger equation

$$(\hat{H} - E)\psi(x, y) = 0 \tag{5.3}$$

defines the quantum-mechanical motion ($\hat{H}$ is the quantum-mechanical version of the Hamiltonian $\mathcal{H}$ defined in (5.1)).

We begin by applying the semiclassical methods available for integrable systems. Since the problem is separable the application of the semiclassical EBK (Einstein, Brillouin, Keller) quantization [51] is straightforward. The problem reduces to two one-dimensional problems, and the action corresponding to each of them is quantized. For the motion along the y axis (parallel to the boundary) the action I_y is

$$I_y = \frac{1}{2\pi}\oint p_y \, dy = \frac{p_y L}{2\pi} = n_y \hbar. \tag{5.4}$$

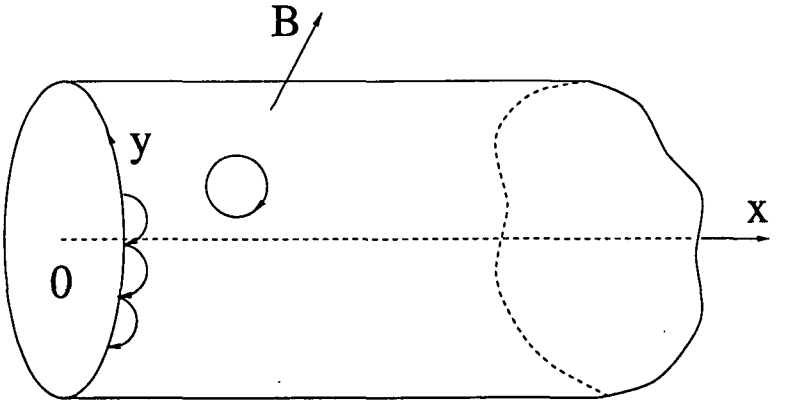

Figure 5.1: Semi-infinite cylinder in the magnetic field B.

The motion along the x axis (perpendicular to the boundary) is different for the bulk and the edge states, therefore their quantization is different too. In particular the energy of the bulk states is obtained from

$$\begin{aligned} I_x &= \frac{1}{2\pi}\oint p_x\,dx = \frac{1}{\pi}\int_0^{2r_c}\sqrt{2mE-(p-\frac{e}{c}Bx)^2}\,dx \\ &= \hbar(n_x+\frac{1}{2}). \end{aligned} \tag{5.5}$$

The integral can be calculated, and gives the usual Landau levels for the unrestricted motion $E=\hbar\omega(n_x+\frac{1}{2})$. For the edge states the EBK condition is

$$\begin{aligned} I_x &= \frac{1}{2\pi}\oint p_x\,dx = \frac{1}{\pi}\int_0^{r_c+\frac{p_y}{m\omega}}\sqrt{2mE-(p_y-\frac{e}{c}Bx)^2}\,dx \\ &= \hbar(n_x+\frac{3}{4}). \end{aligned} \tag{5.6}$$

The two differences between (5.5) and (5.6) are apparent: first the integration range is restricted because of the boundary for the edge integral, second the Maslov index for the edge is $\frac{3}{4}$ instead of $\frac{1}{2}$ for the bulk. This means that the bulk states do not feel the boundary and therefore their energies are degenerate Landau levels. The energies of the edge states are implicit solutions of (5.6), and are non-degenerate. Therefore there is a singularity in the EBK spectrum separating the bulk and edge energies.

5.4 Matching the WKB wavefunctions.

Since the motion in the y direction is trivial, the Schrödinger equation (5.3) together with the boundary condition (5.2) reduces to a one-dimensional Sturm-Liouville

problem. A systematic WKB method is well-developed for those kind of problems and improves the EBK quantization. In particular a WKB function is obtained from several branches each of them being valid in a domain determined by the turning points. These branches are asymptotically matched. The resulting WKB wavefunction is then required to satisfy the boundary condition (5.2), which gives the WKB energies.

Once the variables are separated in the Schrödinger equation (5.3), the one-dimensional Sturm-Liouville problem for the function $\varphi(x) = e^{-\frac{ip_y y}{\hbar}}\psi(x,y)$ is defined by

$$(\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + \frac{1}{2m}(p_y - \frac{eB}{c}x)^2 - E)\,\varphi(x) = 0, \tag{5.7}$$

$\varphi(x)$ satisfying the boundary conditions:

$$\varphi(0) = 0, \tag{5.8}$$

$$\lim_{x\to\infty}\varphi(x) = 0. \tag{5.9}$$

Introducing the dimensionless variable $\tilde{x} = \sqrt{\frac{2m\omega}{\hbar}}x$, equation (5.7) rewrites

$$(\frac{\partial^2}{\partial\tilde{x}^2} + (\frac{E}{\hbar\omega} - \frac{1}{4}(\tilde{x}-\tilde{x}_0)^2))\,\varphi(\tilde{x}) = 0, \tag{5.10}$$

where $x_0 = \frac{p_y c}{eB}$. The subsequent transformation using the variable $\xi = \sqrt{\frac{\epsilon}{2}}(\tilde{x} - \tilde{x}_0) - 1$ gives

$$\epsilon^2 f''(\xi) - (\xi^2 + 2\xi)\,f(\xi) = 0, \tag{5.11}$$

where $\epsilon = \frac{\hbar\omega}{2E}$ and $f(\xi) = \varphi(\tilde{x})$.

For small values of ϵ, this is a standard example of equation where the WKB method is applicable. It has two turning points at $\xi_1 = 0$ and $\xi_2 = -2$. Sufficiently far from them, the WKB function is given by the following asymptotic expression [52]

$$f_{WKB}(\xi) = (\xi^2+2\xi)^{-\frac{1}{4}}\left(c_1 e^{-\frac{1}{\epsilon}\int^{\xi} dt\sqrt{t^2+2t}} + c_2 e^{\frac{1}{\epsilon}\int^{\xi} dt\sqrt{t^2+2t}}\right) \tag{5.12}$$

In the vicinity of the turning points this approximation breaks down. The potential $(\xi^2+2\xi)$ is then linearized and the resulting Airy equation can be solved exactly. The domains of validity of the different branches (5.12) and of the Airy functions overlap, at points where one can match (5.12) with the first term in the asymptotic expansion of the Airy functions [52].

From these matched WKB wavefunctions $f_{WKB}(\xi)$ we can calculate the spectrum by requiring this function to satisfy the boundary condition (5.8). Those energies are solutions of the following implicit equation written in terms of the variable $\xi_0 = \sqrt{\frac{\epsilon}{2}}\tilde{x}_0$

$$f_{WKB}(-\xi_0 - 1) = 0. \tag{5.13}$$

For convenience, we shall consider from now on the energies as functions of ξ_0.

The function $f_{WKB}(\xi)$ is built out of five branches, related to the different intervals of ξ. We start from large ξ's.

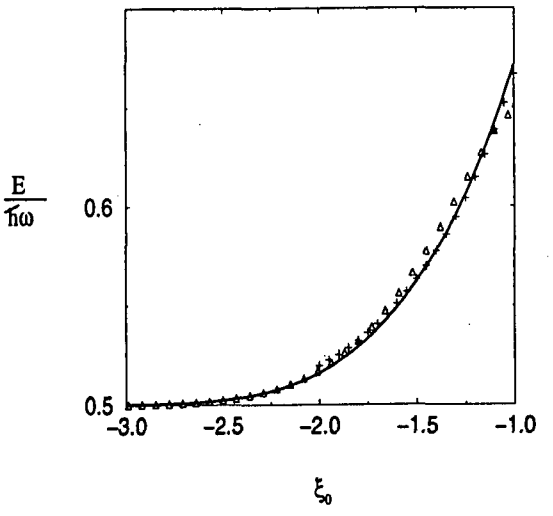

Figure 5.2: The energy spectrum: the full line is the exact spectrum, triangles are the zeros of the second branch and pluses - the zeros of the third branch.

i. The first branch has a domain defined by $\xi \gg \epsilon^{\frac{2}{3}}$ where the expression (5.12) holds. The unknown constants are determined by using the boundary condition at infinity (5.9). This fixes $c_2 = 0$. We set arbitrarily $c_1 = 1$, and we obtain for the first branch of the WKB function

$$f^{(1)}_{WKB}(\xi) = (\xi^2 + 2\xi)^{-\frac{1}{4}}\, e^{-\frac{1}{\epsilon}\int_0^\xi dt\sqrt{t^2+2t}}. \tag{5.14}$$

This function is always nonzero , and therefore does not give any energy solution of (5.13).

ii. The second branch is a solution of the linearized equation (5.11) near the first turning point $\xi_1 = 0$:

$$\epsilon^2 f''(\xi) - 2\xi\, f^{(2)}_{WKB}(\xi) = 0. \tag{5.15}$$

It is therefore valid for $|\xi| \ll 1$. The general solution of the linearized equation (5.15) is a linear combination of the two independent Airy functions. When ξ belongs to the interval $\epsilon^{\frac{2}{3}} \ll \xi \ll \epsilon^{\frac{2}{5}}$, the arguments of the Airy functions are large so that their asymptotic approximations can be used. On the other hand the first branch $f^{(1)}_{WKB}(\xi)$ is still valid in this interval. We match here these two functions, and determine the unknown coefficients by multiplying the Airy functions. This gives for the second branch

$$f^{(2)}_{WKB}(\xi) = \frac{2\sqrt{\pi}}{(2\epsilon)^{\frac{1}{6}}}\,\mathrm{Ai}(\frac{2^{\frac{1}{3}}}{\epsilon^{\frac{2}{3}}}\xi). \tag{5.16}$$

and the energies

$$E = \hbar\omega(\frac{a_i}{2\xi_0 - 2})^{\frac{3}{2}}, \tag{5.17}$$

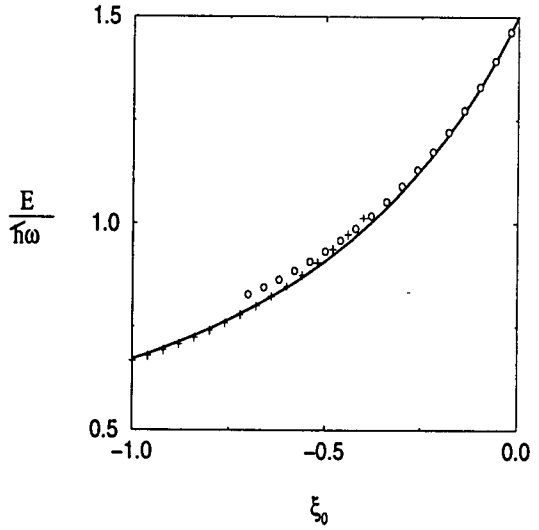

Figure 5.3: The energy spectrum: circles are the zeros of the fourth branch, otherwise notations as previously.

where a_i is the i'th zero of the Airy function. This zero gives the i'th energy branch corresponding to the i'th Landau level for the free particle case. Another thing to be noted from Eq.(5.17) is that there are no energies for $\xi_0 > 1$, since the real zeros of the Airy function are negative.

iii. Between the two turning points ξ_1 and ξ_2 the expression (5.12) holds again and to fix it precisely we do the matching with $f^{(2)}_{WKB}(\xi)$ in the interval $-\epsilon^{\frac{2}{5}} \ll \xi \ll -\epsilon^{\frac{2}{3}}$ which gives

$$f^{(3)}_{WKB}(\xi) = 2(-\xi^2 - 2\xi)^{-\frac{1}{4}} \sin(\frac{1}{\epsilon}\int_{\xi}^{0} dt\,\sqrt{-t^2-2t} + \frac{\pi}{4}). \tag{5.18}$$

The argument of the sine is non-negative, therefore only non-negative zeros will give energies. After integration we obtain using (5.13) an implicit equation for the energies

$$\frac{1}{\epsilon}(\frac{\pi}{4} + \frac{1}{2}\arcsin\xi_0 + \frac{1}{2}\xi_0\sqrt{1-\xi_0^2}) = \frac{3\pi}{4} + n\pi, \tag{5.19}$$

where n is a positive integer. We note that this condition is exactly the EBK quantization rule for the edge states (5.6). The comparison of the energies derived within the WKB approximation with the exact ones is shown in fig. 5.2.

iv. This branch represents the function in the vicinity of the second turning point $\xi_2 = -2$. Repeating the scheme of matching with the previous third branch,

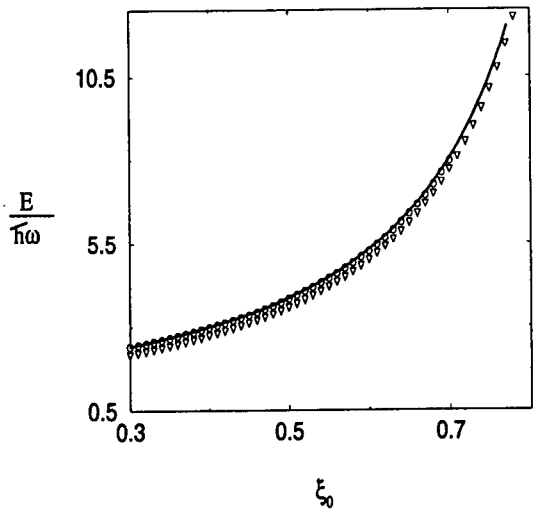

Figure 5.4: The energy spectrum: triangles are the zeros of the fifth branch, otherwise notations as previously.

we obtain:

$$f^{(4)}_{WKB}(\xi) = \frac{2\sqrt{\pi}}{(2\epsilon)^{\frac{1}{6}}}\left(\sin\frac{\pi}{2\epsilon}\mathrm{Ai}(-\frac{2^{\frac{1}{3}}}{\epsilon^{\frac{2}{3}}}(\xi+2))\right.$$
$$\left.+\cos\frac{\pi}{2\epsilon}\mathrm{Bi}(-\frac{2^{\frac{1}{3}}}{\epsilon^{\frac{2}{3}}}(\xi+2))\right). \qquad (5.20)$$

Inserting it in (5.13) gives the energies due to the fourth branch. They are shown together with the solutions of (5.19) and the exact energies in fig. 5.3.

v. The fifth branch $f^{(5)}_{WKB}(\xi)$ is derived in a similar way, i.e. for $\xi \ll -\epsilon^{\frac{2}{3}} - 2$:

$$f^{(5)}_{WKB}(\xi) = (\xi^2+2\xi)^{-\frac{1}{4}}\left(\sin(\frac{\pi}{2\epsilon})e^{-\frac{1}{\epsilon}\int_{\xi}^{-2}dt\sqrt{t^2+2t}}\right.$$
$$\left.+2\cos(\frac{\pi}{2\epsilon})e^{\frac{1}{\epsilon}\int_{\xi}^{-2}dt\sqrt{t^2+2t}}\right). \qquad (5.21)$$

The equation to be solved for the energies is

$$\frac{1}{2}\tan\frac{\pi}{2\epsilon} = e^{\frac{1}{\epsilon}(-\mathrm{arccosh}(-\xi_0)-\xi_0\sqrt{\xi_0^2-1})}. \qquad (5.22)$$

When $|\xi_0|$ is large the right-hand side of this equation is also a large number. The energies are given to a good approximation by the arguments of tangent at points where it diverges. The energies thus obtained are

$$\frac{1}{2\epsilon} = n_x + \frac{1}{2},$$

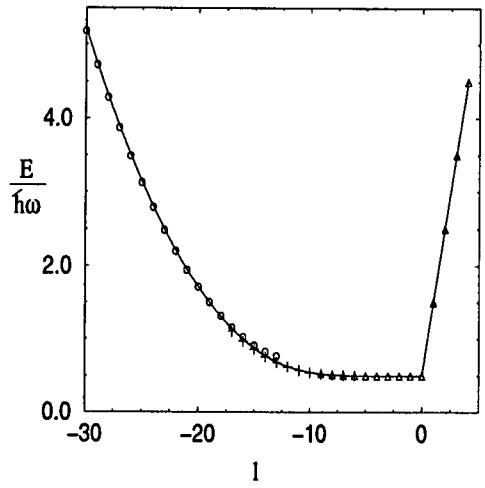

Figure 5.5: The energy spectrum of the disc as function of the kinetic momentum ($N_\Phi = 20$): circles are the zeros of the third branch, pluses - the zeros of the fourth branch and triangles are the zeros of the fifth branch.

i.e. are exactly the energies of the bulk states within the EBK quantization. The solutions of the energy equations for the fourth and the fifth branches and their comparison with exact energies is shown in fig. 5.4.

On the figures 5.2, 5.3 and 5.4 we notice the very good agreement between the exact calculation and the matched WKB approximation even for the lowest energies. The distinction between the bulk and the edge states disappears within this approximation, and the spectrum rises smoothly from $\frac{\hbar\omega}{2}$ (from above) to infinitely large energies.

5.5 Semiclassical spectrum of the disc in the magnetic field.

It is possible to generalize the previous analysis to the study of another integrable billiard: the disc in a uniform magnetic field (the full account of this work is presented in [53]).

The Schrödinger equation is written in polar coordinates, and the conserved angular momentum will be denoted by l. Therefore the non-trivial problem is to solve the radial equation which in convenient units is

$$\left(\epsilon^2\left(\frac{d^2}{d\xi^2}+\frac{1}{\xi}\frac{d}{d\xi}\right)-\frac{\xi^2}{4}+1-l_z-\frac{l_z^2}{\xi^2}\right)\varphi(\xi)=0, \tag{5.23}$$

here $\xi=\frac{r}{r_c}$, $\epsilon=\hbar\omega/2E$ and $l_z=l\epsilon$. The radial part of the wavefunction is $\varphi(\xi)$.

Because of the singularity at the origin due to the centrifugal potential l_z^2/ξ^2 in equation (5.23), the WKB method can not be applied directly. We go around this obstacle by making the following change of variable, $x = -\ln(\xi^2/a)$ [54], where $a = 2(1 - l_z)$. The resulting equation for the function $f(x) = \varphi(\xi)$ is:

$$(\frac{4\epsilon}{a})^2 \frac{d^2 f}{dx^2} = Q(x) f(x), \quad Q(x) = e^{-2x} - 2e^{-x} + (\frac{2l_z}{a})^2. \tag{5.24}$$

This equation can be solved using a WKB analysis similar to that of the previous section. The two turning points are $x_\pm = -\ln(1 \mp c)$, where $c = \sqrt{1 - (2l_z/a)^2}$. However another problem arises - for certain values of the parameter l_z the two turning points get so close one to another, that the method does not really work. We use therefore a better method, the so-called comparison equation method [55]. The idea is to start with the matched WKB function, which we constructed in the previous section, then to multiply it by a slowly varying amplitude and to stretch or contract its argument (by introducing a mapping function). Substituting the modified wavefunction into (5.24), an equation for the mapping function is obtained, which can be solved by a semi-classical approximation.

The five branches of the WKB approximation to the function $f(x)$ are given by

$$\begin{aligned}
& f_{WKB}(x) \\
& = Q(x)^{-\frac{1}{4}} e^{\frac{i}{\hbar}\pi I_r(x)}, \quad \text{if } -e^{-x} + 1 - c \gg \eta \\
& = \frac{2\sqrt{\pi}}{(c - c^2)^{\frac{1}{6}}} (\frac{a}{8\epsilon})^{\frac{1}{6}} \mathrm{Ai}\left((\frac{a\sqrt{2c}}{4\epsilon(1-c)})^{\frac{2}{3}} (-e^{-x} + 1 - c) \right), \quad \text{if } |e^{-x} - 1 + c| \ll c \\
& = 2(-Q(x))^{-\frac{1}{4}} \sin\left(\frac{\pi I_r(x)}{\hbar} + \frac{\pi}{4} \right), \quad \text{if } e^{-x} - 1 + c \gg \eta,\ -e^{-x} + 1 + c \gg \eta \\
& = \frac{2\sqrt{\pi}}{(c + c^2)^{\frac{1}{6}}} (\frac{a}{8\epsilon})^{\frac{1}{6}} \left\{ \sin(\frac{\pi}{2\bar{\epsilon}}) \mathrm{Ai}\left((\frac{a\sqrt{2c}}{4\epsilon(1+c)})^{\frac{2}{3}} (e^{-x} - 1 - c) \right) + \right. \\
& \quad \left. + \cos(\frac{\pi}{2\bar{\epsilon}}) \mathrm{Bi}\left((\frac{a\sqrt{2c}}{4\epsilon(1+c)})^{\frac{2}{3}} (e^{-x} - 1 - c) \right) \right\} \quad \text{if } |e^{-x} - 1 - c| \ll c \\
& = Q(x)^{-\frac{1}{4}} \left\{ \sin(\frac{\pi}{2\bar{\epsilon}}) e^{-\frac{i}{\hbar}\pi I_r(x)} + 2\cos(\frac{\pi}{2\bar{\epsilon}}) e^{\frac{i}{\hbar}\pi I_r(x)} \right\}, \quad \text{if } e^{-x} - 1 - c \gg \eta
\end{aligned} \tag{5.25}$$

Here η is a small parameter, and $\bar{\epsilon}$ satisfies

$$\frac{1}{2\bar{\epsilon}} = \frac{1}{2\epsilon} - l\,\theta(l), \tag{5.26}$$

(where $\theta(l) = 0$ if $l < 0$ and 1 if $l \geq 0$). The classical radial action $I_r(x)$ is

$$\begin{aligned}
& \frac{4\pi}{am\omega r_c^2} I_r(x) = \\
& \sqrt{c^2 - (e^{-x} - 1)^2} + \arccos(\frac{1 - e^{-x}}{c}) - \sqrt{1 - c^2}\, \arccos(\frac{1 - c^2}{c} e^x - \frac{1}{c})
\end{aligned} \tag{5.27}$$

The numerical calculation using (5.25) shows a clean agreement with the exact spectrum - *even* for the lowest Landau level (see figure 5.5). Indeed we are able

to construct the semi-classical spectra of the integrable magnetic billiards to a high accuracy. The spectrum is composed of several branches, which can be associated with bulk or edge states.

Chapter 6

Heat kernel of billiards in a uniform magnetic field.

6.1 Introduction.

In this chapter we pursue the discussion of the spectral properties of integrable magnetic billiards. However in contrast to the previous chapter, where the emphasis was put on a precise calculation of the energies, we shall consider here the smooth, asymptotic spectral properties. Whereas it is important to know the spectrum with a sufficient precision in order to describe low-temperature and high magnetic field phenomena, such as the Quantum Hall effect (as was argued in the previous chapter), the high temperature and (or) the weak magnetic field response, like for instance the orbital diamagnetism is often determined by smoothed spectral quantities (we will have to say more on this in the next chapter). We shall describe them here by defining and calculating the heat kernel or equivalently its Laplace transform. The small time asymptotic expansion of the heat kernel is simply related to the smooth part of the density of states (the so-called Weyl expansion) [56] and to smoothed thermodynamic quantities like the magnetization [57]. This asymptotic expansion of the heat kernel for the semi-infinite plane gives the perimeter correction to the Landau diamagnetism as noted by Robnik [58]. We shall expand the heat kernel in two different ways obtaining the same results which differ however from those obtained by Robnik. We subsequently compare our results with those obtained by using the Balian-Bloch [10] expansion. We show in agreement with previous results [59] that this last method is not very convenient in the presence of a magnetic field due to the fact that it does not give rise to a well defined expansion since all higher corrections do not vanish and can not be neglected. Another asymptotic method we use, following Stewartson and Waechter [60], is powerful enough to give in principle all the asymptotic series for the semi-infinite plane in a magnetic field. We argue that all the coefficients in these series are universal in a sense that we shall precise.

6.2 The resolvent of a bounded system.

Before starting the asymptotic analysis, we need to derive an exact expression for the resolvent associated to the motion of an electron in a system with a boundary and in a magnetic field.

6.2.1 An exact expression for the resolvent

The resolvent is defined by:

$$G(E) = \mathrm{Tr}\,\frac{1}{\mathrm{E}+\hat{\mathrm{H}}} = \sum_{\mathrm{n}} \frac{1}{\mathrm{E}+\mathrm{E_n}}. \tag{6.1}$$

It is a central quantity to study the spectral and thermodynamic properties as we shall see in the following. It was extensively studied for the problem of the Laplacian on manifolds [61, 62] with boundaries and in particular its Laplace transform (the heat kernel) gives in the asymptotic limit the Weyl expansion for the density of states. We consider the semi-infinite plane case in a uniform magnetic field. The resolvent does not have any singularity in energies for $E \geq 0$, except at infinity. To obtain the asymptotic expansion for large E we shall extend to the magnetic case the method developed in the work of Stewartson and Waechter [60].

The resolvent $G(E)$ satisfies the equation:

$$(\hat{H}+E)G(E,\mathbf{r},\mathbf{r}') = \delta(\mathbf{r}-\mathbf{r}'). \tag{6.2}$$

Since the momentum in the y direction is conserved, this equation can be reduced to a one-dimensional Sturm-Liouville problem using the Fourier transform

$$G(E,\mathbf{r},\mathbf{r}') = \frac{1}{2\pi\hbar}\int_{-\infty}^{\infty} dp\, e^{\frac{ip(y-y')}{\hbar}}\, G_p(E,x,x') \tag{6.3}$$

which satisfies (compare with (5.7)):

$$(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + \frac{1}{2m}(p-\frac{eB}{c}x)^2 + E)\, G_p(E,x,x') = \delta(x-x') \tag{6.4}$$

(where we used the identity $\delta(y-y') = \int_{-\infty}^{\infty} dp\, e^{\frac{ip(y-y')}{\hbar}}$). In the variable $\tilde{x}$, the equation is further transformed to (compare with (5.10)

$$(\frac{\partial^2}{\partial\tilde{x}^2} + (-\frac{E}{\hbar\omega} - \frac{1}{4}(\tilde{x}-\tilde{x}_0)^2))(-\frac{\hbar^2}{2m}\sqrt{\frac{2m\omega}{\hbar}}G_p(E,\tilde{x},\tilde{x}')) = \delta(\tilde{x}-\tilde{x}'). \tag{6.5}$$

Finally, defining the variable $\eta = \tilde{x} - \tilde{x}_0$, we obtain the Weber equation:

$$f''(\eta) + (\nu + \frac{1}{2} - \frac{1}{4}\eta^2)\, f(\eta) = \delta(\eta-\eta') \tag{6.6}$$

(where $\nu = -\frac{E}{\hbar\omega} - \frac{1}{2}$). The two independent solutions are the parabolic cylinder (Weber) functions $D_\nu(\eta), D_\nu(-\eta)$ (with a Wronskian equal to $\frac{\sqrt{2\pi}}{\Gamma(-\nu)}$). The Green's function which satisfies (6.6) and vanishes for a diverging $|\eta|$ is

$$\frac{\hbar^2}{2m}\sqrt{\frac{2m\omega}{\hbar}}G_p^\infty(E,\eta,\eta') = \frac{\Gamma(-\nu)}{\sqrt{2\pi}}D_\nu(\eta_>)D_\nu(-\eta_<). \tag{6.7}$$

It gives the Green's function for the particle in the infinite plane with a uniform magnetic field.

We need the resolvent for the particle in the semi-infinite plane. To obtain the Green's function which satisfies Dirichlet boundary conditions at $\eta = -\tilde{x}_0$, we add to $G_p^\infty(E,\eta,\eta')$ a solution of the homogeneous Weber's equation which makes the sum to vanish on the boundary

$$\frac{\hbar^2}{2m}\sqrt{\frac{2m\omega}{\hbar}}G_p(E,\eta,\eta') = \frac{\Gamma(-\nu)}{\sqrt{2\pi}}(D_\nu(\eta_>)D_\nu(-\eta_<) - \frac{D_\nu(\tilde{x}_0)}{D_\nu(-\tilde{x}_0)}D_\nu(\eta_>)D_\nu(\eta_<)). \tag{6.8}$$

The resolvent is then given by:

$$G(E) = \int_0^\infty dx \int_0^L dy\, G(E,\mathbf{r},\mathbf{r}') =$$

$$\int_0^\infty dx \int_0^L dy \int_{-\infty}^\infty \frac{dp}{\pi\hbar^2}\sqrt{\frac{m}{4\pi\hbar\omega}}\,\Gamma(-\nu)\,(D_\nu(\eta)D_\nu(-\eta) - \frac{D_\nu(\tilde{x}_0)}{D_\nu(-\tilde{x}_0)}D_\nu^2(\eta)). \tag{6.9}$$

The integrand does not depend on y, therefore the integral over y is equal to L, the length of the boundary.

It is interesting to extract the infinite plane part of the resolvent, corresponding to the free electron motion in the magnetic field. In order to work with a meromorphic function, we regularize $G^\infty(E)$ by subtracting its value at the energy $E = \frac{\hbar\omega}{2}$

$$G^\infty(E) - G^\infty(E = \frac{\hbar\omega}{2}) = L^2 \int_{-\infty}^\infty d\eta \frac{m}{2(2\pi)^{\frac{1}{2}}\hbar^2}(\Gamma(-\nu)D_\nu(\eta)D_\nu(-\eta) -$$

$$\Gamma(-\nu=1)D_{\nu=-1}(\eta)D_{\nu=-1}(-\eta)) = -L^2\frac{m}{4\pi\hbar^2}\left(\Psi(-\nu) - \Psi(1)\right). \tag{6.10}$$

where $\Psi(-\nu) = -\frac{\Gamma'(-\nu)}{\Gamma(-\nu)}$, and $\int_0^\infty dx$ is taken to be equal to $\frac{L}{2}$.

The boundary term of the resolvent (6.9) is then given by

$$G(E) - G^\infty(E) = -\frac{L\Gamma(-\nu)}{2\pi\hbar}\sqrt{\frac{m}{4\pi\hbar\omega}}\int_{-\tilde{x}_0}^\infty d\eta \int_{-\infty}^\infty d\tilde{x}_0 \frac{D_\nu(\tilde{x}_0)}{D_\nu(-\tilde{x}_0)}D_\nu^2(\eta)$$

$$= \frac{L\Gamma(-\nu)}{2\pi\hbar}\sqrt{\frac{m}{4\pi\hbar\omega}}\int_{-\infty}^\infty d\tilde{x}_0 \frac{D_\nu(\tilde{x}_0)}{D_\nu(-\tilde{x}_0)}(D_\nu(-\tilde{x}_0)\frac{\partial}{\partial\nu}D_\nu{}'(-\tilde{x}_0)$$

$$-D_\nu{}'(-\tilde{x}_0)\frac{\partial}{\partial\nu}D_\nu(\tilde{x}_0)) \tag{6.11}$$

(for the integral with respect to η see [63]). We finally obtain

$$G(E) - G^{\infty}(E = \frac{\hbar\omega}{2}) = L^2 \frac{m}{4\pi\hbar^2}\Psi(1) - \sqrt{\frac{mL^2}{8\pi^2\hbar^3\omega}} \int_{-\infty}^{\infty} d\tilde{x}_0 \frac{\frac{\partial}{\partial\nu}(D_\nu(-\tilde{x}_0))}{D_\nu(-\tilde{x}_0)}. \quad (6.12)$$

There is another (shorter) way to obtain the relation (6.12). The integrated density of states (the counting function) in a quantum system can be expressed through the usual Green's operator:

$$N(E) = \sum_n \oint \frac{d\epsilon}{2\pi i} \frac{1}{\epsilon - E_n} = -\oint \frac{d\epsilon}{2\pi i} \mathrm{Tr}\, \hat{\mathcal{G}}(\epsilon), \quad (6.13)$$

where $\hat{\mathcal{G}}(\epsilon) = \frac{1}{\hat{H}-\epsilon}$ is the Green's operator. The contour encircles the energy poles in the complex ϵ plane. It is important to emphasize that (6.13) is true only for meromorphic functions. If $\mathrm{Tr}\, \hat{\mathcal{G}}(\epsilon)$ is not a meromorphic function (as in the problem of unbounded motion in a magnetic field) it should be made such by appropriate modifications. This can always be done as guaranteed by the theorem of Mittag-Lefler [64].

Suppose now that we arrived to a formula of the type

$$N(E) = \oint \frac{d\epsilon}{2\pi i} f(\epsilon), \quad (6.14)$$

where $f(\epsilon)$ some function (it appears that such a relation can always be written, at least formally, for a separable system). Then, comparing equations (6.13) and (6.14) we obtain that

$$\mathrm{Tr}\, \hat{\mathcal{G}}(\epsilon) = -f(\epsilon). \quad (6.15)$$

Our resolvent $G(E)$ is simply the trace of the Green's operator taken with the negative argument. Therefore it is given by:

$$G(E) = -f(-E). \quad (6.16)$$

Let us illustrate how a relation of the type (6.14) can be obtained for the case of a semi-infinite plane and a uniform magnetic field.

The energies of the stationary states are obtained requiring that the wave function satisfies the boundary condition (5.2). Since they are the parabolic cylinder functions, the equation to be solved to find the energies is

$$D_{\frac{\epsilon}{\hbar\omega}-\frac{1}{2}}\left(-\sqrt{\frac{2m\omega}{\hbar}} \cdot \frac{pc}{eB}\right) = 0, \quad (6.17)$$

where $p = 2\pi\frac{\hbar n}{L}$, and n is an integer. The integrated density of states is equal to the number of zeros of the parabolic cylinder function with the index belonging to the interval $[-\frac{1}{2}, \frac{E}{\hbar\omega} - \frac{1}{2}]$. The number of zeros of an analytic function in some region of the complex plane is given by the following relation from complex analysis [64]:

$$N(E) = \sum_n \oint \frac{d\epsilon}{2\pi i} \frac{\frac{d}{d\epsilon} D_{\frac{\epsilon}{\hbar\omega}-\frac{1}{2}}\left(-\sqrt{\frac{2m\omega}{\hbar}} \cdot \frac{pc}{eB}\right)}{D_{\frac{\epsilon}{\hbar\omega}-\frac{1}{2}}\left(-\sqrt{\frac{2m\omega}{\hbar}} \cdot \frac{pc}{eB}\right)}, \quad (6.18)$$

where the integration contour encircles zeros of the parabolic cylinder function.

Changing the sum into an integral we obtain:

$$N(E) = \int_{-\infty}^{\infty} dn \oint \frac{d\epsilon}{2\pi i} \frac{\frac{d}{d\nu} D_{\nu-\frac{1}{2}}\left(-\sqrt{\frac{2\hbar}{m\omega}} \cdot \frac{2\pi n}{L}\right)}{D_{\nu-\frac{1}{2}}\left(-\sqrt{\frac{2\hbar}{m\omega}} \cdot \frac{2\pi n}{L}\right)} \frac{1}{\hbar\omega}. \tag{6.19}$$

which has the form (6.14) and therefore the relation (6.16) can be applied to find the resolvent $G(E)$. Again one should keep in mind that the application of the formula (6.15) is only possible after the resolvent is transformed in order to be a meromorphic function. Using the regularization as previously and making a change of the integration variable we rederive the formula (6.12) for the resolvent $G(E)$.

This argument extends to any separable system. As an example we derive here the resolvents of a particle moving in a disk, with and without magnetic field.

Consider a particle confined to a disc of radius R. Introducing the momentum $k^2 = \frac{2mE}{\hbar^2}$, the energies are solutions of the equation

$$J_l(kR) = 0, \tag{6.20}$$

where l is the angular momentum quantum number. The number of zeros is equal to the integral of the logarithmic derivative of the Bessel function:

$$N(E) = \sum_l \oint \frac{d\epsilon}{2\pi i} \frac{\frac{d}{d\epsilon} J_l(kR)}{J_l(kR)}. \tag{6.21}$$

Then according to our method, we obtain the resolvent

$$G(E) = \sum_l \frac{m}{\hbar^2 k} \cdot \frac{\frac{d}{dk} I_l(kR)}{I_l(kR)}. \tag{6.22}$$

which gives the result of Stewartson and Waechter [60] after subtracting the resolvent corresponding to the infinite plane.

In the presence of a magnetic field, the energy of the particle moving in a circular billiard is given by

$${}_1F_1\left(\frac{l+|l|+1}{2} - \frac{E}{\hbar\omega}; 1+|l|; N_\Phi\right) = 0, \tag{6.23}$$

where $N_\Phi = \frac{SB}{\Phi_0}$ is the number of flux quanta per total area. The counting function is now

$$N(E) = \sum_l \oint \frac{d\epsilon}{2\pi i} \frac{\frac{d}{d\epsilon} {}_1F_1\left(\frac{l+|l|+1}{2} - \frac{\epsilon}{\hbar\omega}; 1+|l|; N_\Phi\right)}{{}_1F_1\left(\frac{l+|l|+1}{2} - \frac{\epsilon}{\hbar\omega}; 1+|l|; N_\Phi\right)}. \tag{6.24}$$

and the resolvent is

$$G(E) = \sum_l \frac{\frac{d}{dE} {}_1F_1\left(\frac{l+|l|+1}{2} + \frac{E}{\hbar\omega}; 1+|l|; N_\Phi\right)}{{}_1F_1\left(\frac{l+|l|+1}{2} + \frac{E}{\hbar\omega}; 1+|l|; N_\Phi\right)}. \tag{6.25}$$

we emphasize again that in order to work with well-defined quantities we must subtract from this expression the part of the resolvent corresponding to the infinite plane.

6.2.2 The asymptotic expansion of the resolvent.

We shall derive now an asymptotic expression for the resolvent which, as we shall see, provides a convenient description of the thermodynamic response for a smoothed spectrum. We rewrite the expression (6.12) for the resolvent under the following form:

$$G(E) - G^{\infty}(E = \frac{\hbar\omega}{2}) = L^2 \frac{m}{4\pi\hbar^2}\psi(1) - \sqrt{\frac{mL^2}{8\pi^2\hbar^3\omega}}\frac{\partial}{\partial\nu}(\int_{-\infty}^{\infty} d\tilde{x}_0 \ln D_\nu(\tilde{x}_0)). \quad (6.26)$$

For large positive energies (large negative ν) and large $\tilde{x}_0$ the Darwin asymptotic expansion of the parabolic cylinder function [65, 8] gives:

$$\ln D_\nu(\tilde{x}_0) \sim \frac{\ln 2\pi}{4} - \frac{1}{2}\ln\Gamma(-\nu) + (-\theta(\tilde{x}_0, a) + v(\tilde{x}_0, a)), \quad (6.27)$$

with

$$\theta(\tilde{x}_0, a) = \frac{\tilde{x}_0}{4}\sqrt{\tilde{x}_0^2 + 4a} + a\sinh^{-1}\frac{\tilde{x}_0}{2\sqrt{a}}$$

and

$$v(\tilde{x}_0, a) \sim -\frac{1}{4}\ln(\tilde{x}_0^2 + 4a) + \sum_{s=1}(-1)^s \frac{d_{3s}}{(\sqrt{\tilde{x}_0^2 + 4a})^{3s}},$$

where $a = \frac{E}{\hbar\omega} > 0$, and $\tilde{x}_0^2 + 4a \gg 1$.

The coefficients d_{3s} are odd functions of $\tilde{x}_0$ for odd values of s and even functions of $\tilde{x}_0$ for even s. Since we integrate in (6.16) over all real $\tilde{x}_0$, only even functions of $\tilde{x}_0$ contribute. We obtain for the first three even-indexed coefficients d_{3s} [65]:

$$\begin{aligned} d_6 &= \frac{3}{4}\tilde{x}_0^2 - 2a \\ d_{12} &= \frac{153}{8}\tilde{x}_0^4 - 186a\tilde{x}_0^2 + 80a^2 \\ d_{18} &= \frac{6381}{4}\tilde{x}_0^6 - 29862a\tilde{x}_0^4 + 62292a^2\tilde{x}_0^2 - \frac{31232}{3}a^3. \end{aligned} \quad (6.28)$$

Then the asymptotic expansion of the resolvent $G(E)$ is obtained inserting Darwin expansion (6.27) in the equation (6.26)

$$G(E) - G^{\infty}(E = \frac{\hbar\omega}{2}) \sim L^2 \frac{m}{4\pi\hbar^2}\psi(1) + \sqrt{\frac{mL^2}{32\pi^2\hbar^3\omega}}\frac{\partial}{\partial\nu}(\int_{-\infty}^{\infty} d\tilde{x}_0 \ln\Gamma(-\nu)) +$$

$$\sqrt{\frac{mL^2}{128\pi^2\hbar^3\omega}}\frac{\partial}{\partial\nu}(\int_{-\infty}^{\infty} d\tilde{x}_0 \ln(\tilde{x}_0^2 + 4a)) - \sum_{s=1}\sqrt{\frac{mL^2}{8\pi^2\hbar^3\omega}}\frac{\partial}{\partial\nu}(\int_{-\infty}^{\infty} d\tilde{x}_0 \frac{d_{6s}}{(\sqrt{\tilde{x}_0^2 + 4a})^{3s}}). \quad (6.29)$$

The first two terms give the infinite plane part of the resolvent $G^{\infty}(E)$. Differentiating first in the third term gives:

$$G(E) \sim G^{\infty}(E) - \sqrt{\frac{mL^2}{8\pi^2\hbar^3\omega}}\int_{-\infty}^{\infty} d\tilde{x}_0 \frac{1}{\tilde{x}_0^2 + 4a} +$$

$$\sum_{s=1}\sqrt{\frac{mL^2}{8\pi^2\hbar^3\omega}}\frac{\partial}{\partial a}(\int_{-\infty}^{\infty} d\tilde{x}_0 \frac{d_{6s}}{(\sqrt{\tilde{x}_0^2 + 4a})^{3s}}). \quad (6.30)$$

Performing the integrals order by order in (6.30), we obtain the full asymptotic expansion:

$$G(E) - G^{\infty}(E) \sim -\sqrt{\frac{mL^2}{32\hbar^3\omega}}\frac{1}{\sqrt{a}} + \sqrt{\frac{mL^2}{32\hbar^3\omega}}\left(\frac{9}{256a^{\frac{5}{2}}} - \frac{2625}{262144a^{\frac{9}{2}}} + \frac{241197}{33554432a^{\frac{13}{2}}} - \ldots\right) = -\sqrt{\frac{mL^2}{32\hbar^2}}\left(\frac{1}{\sqrt{E}} - \frac{9(\hbar\omega)^2}{256E^{\frac{5}{2}}} + \frac{2625(\hbar\omega)^4}{262144E^{\frac{9}{2}}} - \frac{241197(\hbar\omega)^6}{33554432E^{\frac{13}{2}}} + \ldots\right) \tag{6.31}$$

This expansion could in principle be continued indefinitely, once the coefficients d_{6s} are known.

6.3 Generalities on the heat kernel.

The heat kernel is defined by [61, 62]

$$P(t) = \mathrm{Tr}\, e^{-\hat{H}t/\hbar} = \sum_{n} e^{-E_n t/\hbar}. \tag{6.32}$$

The Laplace transform of the heat kernel is the resolvent given by expression (6.1). This function is more carefully defined by subtracting its divergent part, which defines the regularized resolvent [56]

$$g(s) = \lim_{N\to\infty}\left[\frac{1}{s^2+E_n} - \frac{mS}{2\pi\hbar^2}\log\left\{\frac{E_N}{s^2}\right\}\right]. \tag{6.33}$$

where S is the area of the two-dimensional system. The large-s asymptotic expansion of $g(s)$ implies the asymptotic expansion for the density of states. By assuming

$$g(s) \sim \sum_{r=1}^{\infty}\frac{c_r}{s^r}. \tag{6.34}$$

the density of states $\rho(E)$ is related to the regularized resolvent defined through (6.33):

$$\rho(E) = \sum_{n=1}^{\infty}\delta(E-E_n) = \frac{mS}{2\pi\hbar^2} - \frac{1}{\pi}\lim_{\epsilon\to 0}\mathrm{Im}\, g(i\sqrt{E-i\epsilon}). \tag{6.35}$$

Then, the large-s asymptotic expansion of the density of states can be obtained using (6.34)

$$\begin{aligned}\rho(E) &\sim \frac{mS}{2\pi\hbar^2} - \frac{1}{\pi}\mathrm{Im}\lim_{\epsilon\to 0}\frac{c_1}{i\sqrt{E-i\epsilon}} - \frac{1}{\pi}\mathrm{Im}\lim_{\epsilon\to 0}\frac{-c_2}{E-i\epsilon} \\ &\quad -\frac{1}{\pi}\mathrm{Im}\lim_{\epsilon\to 0}\frac{-c_3}{i(E-i\epsilon)\sqrt{E-i\epsilon}} - \ldots \\ &= \frac{mS}{2\pi\hbar^2} + \frac{1}{\pi}\frac{c_1}{\sqrt{E}} + \frac{1}{\pi\sqrt{E}}\sum_{r=1}^{\infty}\frac{(-1)^r}{E^r}c_{2r+1}.\end{aligned} \tag{6.36}$$

We note that even powers of s do not contribute to this asymptotic expansion.

As an example we calculate the heat kernel associated to the Landau spectrum for a particle moving in the two-dimensional plane in a uniform magnetic field. The energies are Landau levels $E_n = \hbar\omega\left(n + \frac{1}{2}\right)$, with a degeneracy $N_\Phi = \frac{SB}{\Phi_0}$. The sum in (6.32) can be performed exactly and we obtain the closed expression:

$$P_\infty(t) = \frac{N_\Phi}{2\sinh\frac{\omega t}{2}}. \tag{6.37}$$

The small t asymptotic expansion of the heat kernel is given in this case by the Taylor series of the hyperbolic sine

$$P_\infty(t) \sim \frac{N_\Phi}{\omega t}\left(1 - \frac{(\omega t)^2}{24} + \ldots\right). \tag{6.38}$$

All the terms except for the first one in the large s expansion of the regularized resolvent are Laplace transforms of the corresponding terms in (6.38).

For the semi-infinite plane, using the asymptotic expansion of the resolvent, we can calculate term by term the asymptotic expansion of the heat kernel for small t, by performing an inverse Laplace transform on (6.31)

$$P(t) - P_\infty(t) \sim -\sqrt{\frac{mL^2}{32t\pi\hbar}}\left(1 - \frac{3t^2\omega^2}{64} + \frac{25t^4\omega^4}{16384} - \ldots\right). \tag{6.39}$$

For $B = 0$ (6.39) gives a correct boundary term in the asymptotic expansion of the heat kernel for the semi-infinite plane. It is more appealing to represent the heat kernel for the semi-infinite plane in the presence of the magnetic field as a function of the two dimensionless parameters: $\tau = \omega t$ and $N_\Phi = \frac{BL^2}{\Phi_0}$ (number of the elementary flux quanta). Then

$$P(t) = \frac{N_\Phi}{\tau}\left(1 - \frac{\tau^2}{24} + \frac{7\tau^4}{5760} - \ldots\right) - \frac{\sqrt{N_\Phi}}{4\sqrt{\tau}}\left(1 - \frac{3\tau^2}{64} + \frac{25\tau^4}{16384} - \ldots\right). \tag{6.40}$$

It is instructive to compare the expression (6.40) with its counterpart at $B = 0$. The heat kernel in the absence of magnetic field is simply obtained from (6.40) by taking in each parenthesis the analytic function of τ to be zero. This suggests that a natural extension of the heat kernel expansion for the two-dimensional shape given for example in [56, 60] to the case of magnetic billiard is to multiply each term by an analytic function of τ. These functions should be universal for all flat two-dimensional billiards with smooth boundaries.

6.4 The Balian-Bloch method.

The small time asymptotic expansion of the Heat Kernel can also be found using a method suggested by Balian and Bloch [10]. It consists in a reformulation of the problem of solving a partial differential equation of elliptic type with Dirichlet (or another) boundary condition in terms of an integral equation of the Fredholm type.

This integral equation is then solved iteratively (Neumann series), and each term in this multiple reflection expansion corresponds to one term in the asymptotic series of the heat kernel, as shown by Balian and Bloch [10].

Suppose then that the generalized Dirichlet problem can be solved in a domain D with a boundary S in the absence of magnetic field:

$$(\triangle - \frac{2mE}{\hbar^2})G(E,\mathbf{r},\mathbf{r}') = -\frac{2m}{\hbar^2}\delta(\mathbf{r}-\mathbf{r}') \tag{6.41}$$

The Green's function can be represented as a sum of two terms:

$$G(E,\mathbf{r},\mathbf{r}') = G^{\infty}(E,\mathbf{r},\mathbf{r}') + G^{S}(E,\mathbf{r},\mathbf{r}'), \tag{6.42}$$

where $G^{\infty}(E,\mathbf{r},\mathbf{r}')$ is the Green's function of the infinite plane, and $G^{S}(E,\mathbf{r},\mathbf{r}')$ is the boundary term which satisfies the differential equation (6.41) for $\mathbf{r}$ in D and the boundary condition

$$G^{S}(E,\mathbf{r},\mathbf{r}') = -G^{\infty}(E,\mathbf{r},\mathbf{r}'), \tag{6.43}$$

for $\mathbf{r}$ on S. This boundary term is expressed in terms of an unknown density $\mu_E(\boldsymbol{\alpha},\mathbf{r})$ as

$$G^{S}(E,\mathbf{r},\mathbf{r}') = \int_S d\sigma_{\alpha}\frac{\partial G^{\infty}(E,\mathbf{r},\boldsymbol{\alpha})}{\partial n_{\alpha}}\mu_E(\boldsymbol{\alpha},\mathbf{r}'), \tag{6.44}$$

and $\mu_E(\boldsymbol{\alpha},\mathbf{r})$ is determined by solving the following Fredholm integral equation:

$$\frac{m}{\hbar^2}\mu_E(\boldsymbol{\beta},\mathbf{r}') = -G^{\infty}(E,\boldsymbol{\beta},\mathbf{r}') - \int_S d\sigma_{\alpha}\frac{\partial G^{\infty}(E,\boldsymbol{\beta},\boldsymbol{\alpha})}{\partial n_{\alpha}}\mu_E(\boldsymbol{\alpha},\mathbf{r}'), \tag{6.45}$$

where $\boldsymbol{\alpha},\boldsymbol{\beta},\ldots$ are arbitrary points on the boundary S, $d\sigma_{\alpha}$ is the boundary differential element, $\frac{\partial}{\partial n_{\alpha}}$ is the normal derivative at the point $\boldsymbol{\alpha}$, with the normal oriented towards the interior of the domain. Solving iteratively the integral equation (6.45) for the density $\mu_E(\boldsymbol{\alpha},\mathbf{r})$ and using equations (6.42) and (6.44), the following multiple reflection expansion is obtained for the Green's function:

$$G(E,\mathbf{r},\mathbf{r}') = G^{\infty}(E,\mathbf{r},\mathbf{r}') - \frac{\hbar^2}{m}\int_S d\sigma_{\alpha}\frac{\partial G^{\infty}(E,\mathbf{r},\boldsymbol{\alpha})}{\partial n_{\alpha}}G^{\infty}(E,\boldsymbol{\alpha},\mathbf{r}') +$$
$$\left(\frac{\hbar^2}{m}\right)^2\int_S d\sigma_{\alpha}d\sigma_{\beta}\frac{\partial G^{\infty}(E,\mathbf{r},\boldsymbol{\alpha})}{\partial n_{\alpha}}\frac{\partial G^{\infty}(E,\boldsymbol{\alpha},\boldsymbol{\beta})}{\partial n_{\beta}}G^{\infty}(E,\boldsymbol{\beta},\mathbf{r}') - \ldots \tag{6.46}$$

This approach was applied in this form to the case with a uniform magnetic field perpendicular to the domain D [58]. However, at each order of the obtained multiple reflection expansion we obtain a term which is not gauge invariant. This problem may be easily corrected by introducing the covariant derivative $\frac{\partial}{\partial n_{\alpha}} - \frac{ie}{\hbar c}A_n(\boldsymbol{\alpha})$ instead of the usual $\frac{\partial}{\partial n_{\alpha}}$. This substitution is of no importance when the gauge is chosen such that the vector potential has no component normal to the boundary (as it happens to be in our problem), but generally should be taken into account.

Let us therefore apply the Balian and Bloch method to the semi-infinite plane in a uniform magnetic field [58], in order to check our solution obtained by using

Stewartson and Waechter method. Following Robnik, we calculate the heat kernel $P(t)$ where $P(t) = \int d\mathbf{r} G(t, \mathbf{r}, \mathbf{r})$ and

$$G(E, \mathbf{r}, \mathbf{r}') = \int_0^\infty e^{-\frac{Et}{\hbar}} G(t, \mathbf{r}, \mathbf{r}') \frac{dt}{\hbar}. \tag{6.47}$$

The multiple expansion for the time-dependent Green's function is

$$G(t, \mathbf{r}, \mathbf{r}') = G^\infty(t, \mathbf{r}, \mathbf{r}') - \frac{\hbar^2}{m} \int_S d\sigma_\alpha \int_0^t d\tau \frac{\partial G^\infty(t-\tau, \mathbf{r}, \boldsymbol{\alpha})}{\partial n_\alpha} G^\infty(\tau, \boldsymbol{\alpha}, \mathbf{r}') + \tag{6.48}$$

$$\frac{\hbar^4}{m^2} \int_S d\sigma_\alpha d\sigma_\beta \int_0^t d\tau_1 \int_0^{\tau_1} d\tau_2 \frac{\partial G^\infty(t-\tau_1, \mathbf{r}, \alpha)}{\partial n_\alpha} \frac{\partial G^\infty(\tau_1 - \tau_2, \alpha, \beta)}{\partial n_\beta} G^\infty(\tau_2, \beta, \mathbf{r}') -$$

where the Green's function for the infinite plane is given by

$$G^\infty(t, \mathbf{r}, \mathbf{r}') = \frac{m\omega}{4\pi\hbar \sinh \frac{\omega t}{2}} e^{-\frac{m\omega}{4\hbar}(\mathbf{r}-\mathbf{r}')^2 \coth \frac{\omega t}{2} + \frac{im\omega}{2\hbar}(y-y')(x+x')}. \tag{6.49}$$

We calculate now the first term (proportional to B^2) in the small magnetic field expansion of the heat kernel. It turns out that the first three boundary-dependent terms in the multiple reflection expansion do contribute to this order. The small B expansion of the one-reflection term begins with:

$$-\frac{L}{8}\sqrt{\frac{2m}{\pi\hbar t}} + \frac{L}{8}\sqrt{\frac{2m}{\pi\hbar t}} \frac{7}{192}\omega^2 t^2,$$

for the two-reflection and three-reflection terms, it is respectively:

$$\frac{L}{8}\sqrt{\frac{2m}{\pi\hbar t}} \frac{3}{192}\omega^2 t^2,$$

and

$$-\frac{L}{8}\sqrt{\frac{2m}{\pi\hbar t}} \frac{1}{192}\omega^2 t^2.$$

Therefore the small magnetic field expansion of the heat kernel begins as follows:

$$P(t) = P^\infty(t) - \frac{L}{8}\sqrt{\frac{2m}{\pi\hbar t}} + \frac{L}{8}\sqrt{\frac{2m}{\pi\hbar t}} \frac{3}{64}\omega^2 t^2 - \dots \tag{6.50}$$

which agrees with the previously obtained result (6.39). This however disagrees with Robnik's calculation [58]. He assumed that in the case of a zero-curvature boundary, the one-reflection term contains all the correction due to the boundary (as it is for the problems with zero magnetic field). In fact as already noted by John and Suttorp [59], higher order terms can not be neglected in calculating physical quantities in the geometry with straight boundaries in the presence of a magnetic field. We also remark that in order to calculate the term proportional to ω^{2n} in the asymptotic expansion of the heat kernel, all the multiple reflection terms up to the $2n+1$'th order have to be taken into account. This result is intuitively appealing. Indeed as the magnetic field increases, the trajectories of the particles bend more and more, so that higher and higher terms in the multiple reflection expansion do contribute.

6.5 Perimeter corrections to the Landau diamagnetism.

The heat kernel previously defined is nothing but the partition function of the electron and is therefore simply related to the magnetic susceptibility. We shall now derive the perimeter corrections to the Landau diamagnetic susceptibility using the expansion (6.50) both for a non-degenerate and a degenerate electron gas, comparing them with the results obtained in [58].

For the non-degenerate case we obtain:

$$\chi \simeq -\frac{N\mu^2}{3kT}\left(1-\frac{l}{16L}\right), \tag{6.51}$$

where N is the number of electrons in the system, $\mu = \frac{e\hbar}{2mc}$ is the Bohr magneton and $l = \sqrt{\frac{\pi\hbar^2}{2mkT}}$ is the de Broglie thermal length. Like in [58] the correction is paramagnetic, but is smaller by one order of magnitude. Our result agrees with numerical calculations [66].

For a degenerate electron gas, the connection between the susceptibility and the partition function is different (see [57]). For a two-dimensional system we obtain at $T = 0$

$$\chi \simeq -\frac{Se^2}{24\pi mc^2}\left(1-\frac{9}{16}\frac{1}{Lk_F}\right), \tag{6.52}$$

where k_F is the Fermi wavevector. Here again the correction is paramagnetic and coincides with perturbative calculations [67] at small field.

The perimeter corrections to the Landau diamagnetism (6.51) and (6.52) are universal, being the largest corrections in a general billiard with a boundary of length L. For a generic billiard, this correction is not the only one, and smaller terms related to the curvature of the boundary should be added.

The properties of the heat kernel of manifolds have been extensively investigated starting (among others) from the work of Kac [61] in order to relate the spectral and geometrical descriptions [62]. Our results could be seen as an extension of these works to the case of magnetic billiards. For the case of a straight boundary, the magnetic field adds an infinite series to the bare perimeter term, which is, in some sense, equivalent to an effective curvature of the boundary. If the boundary has a curvature, another length scale enters the problem, coupling with the cyclotron radius.

A full account of this work is given in [68].

Chapter 7

The Landau diamagnetism revisited.

7.1 The Landau diamagnetism as a smooth magnetic response.

The problem of the response of the free electron gas to a uniform magnetic field is almost a century old. The beginning is the pre-quantum era when it was solved in the framework of classical mechanics. The unexpected (even today) result known as the Bohr-van Leeuwen theorem states that the magnetic response of the classical electron gas is zero. It was even a bigger surprise when Landau proved that quantum mechanics disagrees with this theorem and that a spinless electron gas has a finite diamagnetic response.

There is a sufficiently large number of different derivations of the orbital magnetic susceptibility in the quantum regime and perhaps another one is superfluous. However we feel that this discussion fits the logic of this thesis, since it emphasizes the ubiquity of the need to separate a physical quantity into the smooth and oscillating parts and places the Landau calculation in the realm of the smoothed quantities. In fact the large number of supposedly different ways to obtain the result of Landau stems precisely from the large number of possibilities to smooth something oscillating. Landau himself has derived his formula using the Poisson sum rule [69] (see also [70]), and the standard textbook derivation [71, 72] is based on the use of the Euler-Maclaurin summation formula. Our calculation is inspired by the treatment of this problem by Pippard [73] and should be reducible to it.

Later in this chapter we calculate the Landau diamagnetic response of a free electron gas on three surfaces with a constant curvature - a plane, a sphere and a hyperbolic plane. The orbital magnetic susceptibility in all these three cases is the same.

We start however with a gas of non-interacting electrons moving in an infinite plane in a perpendicular and uniform magnetic field B. The energy levels instead of the continuum for a free particle, collapse for the case of a particle moving in the

magnetic field into the so called Landau levels,

$$E = \hbar\omega(n + 1/2), \tag{7.1}$$

where $\omega = eB/mc$, n is a non-negative integer. Each Landau level possesses a macroscopic degeneracy, usually estimated by the total magnetic flux through the system, measured in the units of elementary flux quantum $N_\Phi = \Phi/\Phi_0$ ($\Phi = BS$, with S the area of the system; $\Phi_0 = hc/e$). For the infinite plane the area is infinite, so is the degeneracy of the Landau level, however one is allowed to consider a finite domain, assuming the energy levels (7.1) with the finite degeneracy (compare with the discussion of the hyperbolic plane case). If however one feels uneasy with these infinities, he/she could have in mind a torus with a magnetic field everywhere perpendicular to its surface, which has the same spectrum with the degeneracy exactly equal to $[N_\Phi]$ (the magnetic field is then quantized). The orbital magnetic response of the electrons is measured by the magnetic susceptibility, a definition of which is

$$\chi = -\lim_{B\to 0} \frac{1}{S}\left(\frac{\partial^2\Omega}{\partial B^2}\right)_\mu, \tag{7.2}$$

where $\Omega(B,\mu)$ is the thermodynamic potential, connected to the grand-canonical partition function $\mathcal{Q}$ via $\Omega = -(1/\beta)\ln\mathcal{Q}$. The thermodynamic potential is not a smooth function of the chemical potential at zero temperature, as we will explicitly show, but it gets smoother as the temperature is raised. The diamagnetism of Landau is the smooth part of the magnetic response and most often the temperature serves as a smoothing agent (for instance in [71]). In this case the magnetic field should not be too large, more precisely the condition $\hbar\omega\beta << 1$ should be satisfied. Correspondingly the Landau diamagnetism is sometimes called "the weak magnetic field response". However it is not obligatory to smooth by raising the temperature. Nothing prevents us from smoothing over the chemical potential at zero temperature. It is possible therefore to measure in principle the Landau diamagnetism even at $T = 0$ and strong magnetic field, provided we know how to smooth the actual response.

In this section we would like to argue that the smoothing for this particular problem - calculating the orbital magnetic susceptibility - can be understood as some kind of average of the exact quantity. This average, as it turns out has to minimize the mean square deviation from the actual quantity, thus basically corresponding to the least squares method.

The quantity we consider is the thermodynamic potential $\Omega(\mu)$ at zero temperature, related to the total energy $E(\mu)$ and the particle number $N(\mu)$

$$\Omega(\mu) = E(\mu) - \mu N(\mu). \tag{7.3}$$

Using the spectrum of the electrons in the magnetic field moving on the torus, we would like now to build the function $\Omega(\mu)$ explicitly. It is convenient to make a following rescaling to more natural units: the thermodynamic potential will be measured in units of $N_\Phi\hbar\omega/2$ and the chemical potential in units of $\hbar\omega/2$. The rescaled quantities will be indicated by tilde. Consider then $-\tilde{\Omega}(\tilde{\mu})$. Naturally the range of

the rescaled chemical potential $\tilde{\mu}$ splits into the pieces between the Landau levels. At each Landau level the reduced thermodynamic potential $\tilde{\Omega}$ changes discontinuously its slope. Thus if $0 \leq \tilde{\mu} \leq 1$, the thermodynamic potential is zero. The next piece is $1 \leq \tilde{\mu} \leq 3$. At the beginning of this interval, $\tilde{\mu} = 1$, the first Landau level is filled, this means the number of electrons is $N(1) = N_\Phi$, their total energy $E(1) = N_\Phi \hbar\omega/2$ and hence the thermodynamic potential is zero. Between the Landau levels, the electron number and the total energy do not change, therefore $-\tilde{\Omega}(\tilde{\mu})$ is a linear function. At the end of the interval, $\tilde{\mu} = 3$, the particle number is $N(3) = 2N_\Phi$, the total energy $E(3) = E(1) + 3N_\Phi\hbar\omega/2$ and correspondingly $-\tilde{\Omega}(3) = 2$. It is easy to derive generally that for $\tilde{\mu}$ in the interval $2n - 1 \leq \tilde{\mu} \leq 2n + 1$, (here n is a positive integer) the rescaled thermodynamic potential is given by

$$-\tilde{\Omega}(\tilde{\mu}) = n\tilde{\mu} - n^2. \tag{7.4}$$

This function is shown graphically in figure 7.1 by the solid line. As was already mentioned, when the chemical potential is exactly equal to the energy of the Landau level, the curve has a discontinuous slope. Between the Landau levels it is a straight line.

Now we need to smooth the thermodynamic potential over the chemical potential. Let $\langle\tilde{\Omega}\rangle$ stand for the smoothed rescaled thermodynamic potential. The smoothed function has to average in some sense the real curve, their difference should be as small as possible for all values of rescaled chemical potential. It is not difficult to notice that there are two curves that have infinitely many common points with the solid line in figure 7.1 (they are shown as two dashed lines). These are parabolas, the first is described by $\tilde{\mu}^2/4$, and the second $\tilde{\mu}^2/4 - 1/4$. The first parabola touches the solid line, representing $\tilde{\Omega}(\tilde{\mu})$ at points $\tilde{\mu} = 2n$, the other one at points $\tilde{\mu} = 2n + 1$. Clearly then $-\langle\tilde{\Omega}(\tilde{\mu})\rangle$ has to be a parabola of the following form

$$-\langle\tilde{\Omega}(\tilde{\mu})\rangle = \frac{1}{4}\tilde{\mu}^2 - c, \tag{7.5}$$

here c has to be some constant satisfying $0 < c < 1/4$.

In order to find the constant c, we need a more precise definition of the average $\langle\tilde{\Omega}\rangle$. We propose to minimize the mean square deviation between the smoothed and exact quantities, i.e.

$$\int_{2n-1}^{2n+1} d\tilde{\mu}\left(\langle\tilde{\Omega}(\tilde{\mu})\rangle - \tilde{\Omega}(\tilde{\mu})\right)^2 = \frac{1}{40} - \frac{c}{3} + 2c^2, \tag{7.6}$$

here it is enough to restrict the integral between two arbitrary adjacent Landau levels, because the integral does not depend on n. Minimizing (7.6), we obtain for the constant $c = 1/12$. Hence

$$-\langle\tilde{\Omega}(\tilde{\mu})\rangle = \frac{1}{4}\tilde{\mu}^2 - 1/12, \tag{7.7}$$

and restoring the usual units, the smoothed thermodynamic potential is found to be

$$\Omega(\mu) = -\frac{Sm\mu^2}{4\pi\hbar^2} + \frac{SB^2e^2}{48\pi mc^2}. \tag{7.8}$$

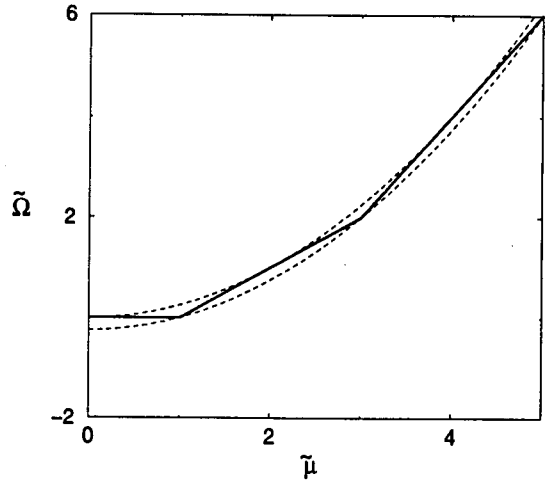

Figure 7.1: Rescaled thermodynamic potential as a function of rescaled chemical potential. The solid line is the exact thermodynamic potential; the dashed lines are two parabolas approximating it.

Using (7.2), we obtain the diamagnetic susceptibility as follows

$$\chi = -\frac{e^2}{24\pi mc^2}. \tag{7.9}$$

This is the usual result of Landau diamagnetism for the two-dimensional system.

The lesson we have learned from this calculation is that the smooth quantity averages in a certain way the exact function, which is singular. From many different averages we find that the least squares method gives a correct answer. This indicates some connection between the asymptotic analysis and the statistical theory to which the method of least squares belongs.

7.2 The derivation of the Landau diamagnetism through the heat kernel formalism.

We would like to present a simple scheme to calculate the smooth part of the chemical potential $\langle\Omega(\mu)\rangle$ (at $T = 0$). It relies on the use of the connection between the chemical potential at zero temperature and the heat kernel, which was developed by Sondheimer and Wilson [57]. We will not prove here this relationship.

Consider the heat kernel, $P(\gamma)$, for the one-particle problem with a Hamiltonian H, defined as follows

$$P(\gamma) = \sum_n e^{-E_n\gamma}, \tag{7.10}$$

here n is the index running over the eigenstates of the Hamiltonian H; E_n are the corresponding energies (in contrast with the definition (6.32), where the time

variable t is used, we prefer here the variable γ with the dimension of inverse energy). As Sondheimer and Wilson show, the thermodynamic potential at zero temperature is simply related to a function $z(E)$, which is defined by means of

$$\frac{P(\gamma)}{\gamma^2} = \int_0^\infty dE\ z(E)e^{-\gamma E}. \tag{7.11}$$

The important result derived in [57] is the following

$$\Omega(\mu) = -z(\mu). \tag{7.12}$$

As was argued in the previous section, the Landau diamagnetism has as its origin the smooth part of the thermodynamic potential, more precisely the magnetic susceptibility can be read off the second term of the large μ asymptotic expansion of $\Omega(\mu)$. Therefore according to (7.12) we have to find the asymptotic behavior of the function $z(E)$ as $E \to \infty$. We will find easier however to calculate the asymptotic expansion of the heat kernel for small γ's. Since the heat kernel is related to $z(E)$ by (7.11), the required asymptotic series of $z(E)$ can be found by inverting this equation.

This scheme can be immediately applied to calculate the magnetic susceptibility for the system considered in the previous section (electrons on the infinite plane in the magnetic field). Using the Landau spectrum with corresponding energies and degeneracies, the heat kernel can be summed up as a closed expression

$$P(\gamma) = \frac{N_\Phi}{2\sinh(\gamma\hbar\omega/2)}. \tag{7.13}$$

Expanding (7.13) for $\gamma \to 0$, we obtain

$$\lim_{\gamma\to 0} P(\gamma) = N_\Phi \left(\frac{1}{\gamma\hbar\omega} - \frac{\gamma\hbar\omega}{24} + \cdots\right). \tag{7.14}$$

The first term in the expansion (7.14) is independent of the magnetic field and corresponds through (7.11) to the first term in the formula (7.8) for the smoothed thermodynamic potential. The leading term in the heat kernel expansion which depends on B is $-N_\Phi\gamma\hbar\omega/24$. It is proportional to γ, and as explained earlier will give the magnetic response. The corresponding term in the large E expansion of the function $z(E)$ is according to (7.11) $-N_\Phi\hbar\omega/24$, we have to change the sign of this expression to obtain the relevant term for the smooth thermodynamic potential. Substituting this expression into (7.2), we again have for the diamagnetic susceptibility

$$\chi = -\frac{e^2}{24\pi mc^2}, \tag{7.15}$$

in agreement with (7.9).

Our scheme is not entirely satisfying, because for instance the third term in the expansion (7.14) when attempted to relate it to a term in the large E expansion of $z(E)$ through (7.11), will give rise to a diverging expression and therefore has no meaning. However it seems that if the two sides of the relationship $z(E)$ converge, they should correctly represent terms in the corresponding asymptotic series. This point requires further study.

7.3 The Landau diamagnetism of the sphere.

In this and the next sections we will examine the magnetic response of the electron gas forming a two-dimensional surface with a constant and finite curvature. First we consider the sphere of radius R (a surface with a constant positive curvature). The magnetic field is perpendicular everywhere to the surface of the sphere and is uniform. It can be associated to a Dirac monopole. We will follow the scheme of the previous section to calculate the magnetic susceptibility. To this end we need the eigenstates with their energies for the one-particle problem on the sphere with the magnetic field. They were obtained by I. Tamm [74] ([75] is a more recent reference). As in the case of the flat torus, the energy levels are labeled by a non-negative index n (called by analogy the Landau levels), and are given by

$$E_n = \hbar\omega(n + \frac{1}{2} + \frac{n(n+1)}{2g}), \tag{7.16}$$

where the dimensionless monopole charge g is defined through $2g = \Phi/\Phi_0$, the total magnetic flux being equal to the product of the magnetic field and the surface area of the sphere $S = 4\pi R^2$. The Dirac quantization condition requires that $2g$ has to be an integer [76] (this point is not essential in what follows). There are $2g + 2n + 1$ eigenstates with energy E_n - the degeneracy of the Landau levels unlike the infinite plane case depends on the index n.

The heat kernel of the sphere is then

$$\begin{aligned} P(\gamma) &= \sum_{n=0}^{\infty}(2g + 2n + 1)e^{-\hbar\omega\gamma(n+1/2+n(n+1)/2g)} \\ &\quad \sum_{n=0}^{\infty}(2g + 2n + 1)e^{-\epsilon_0(2ng+g+n^2+n)}, \end{aligned} \tag{7.17}$$

where the following notation was introduced $\epsilon_0 = \hbar^2/2mR^2$. The asymptotic behavior of the sum in (7.17) as $\gamma \to 0$ should now be found. It turns out that the application of the Euler-Maclaurin summation formula (2.14) to the heat kernel yields the asymptotic expansion. To illustrate the calculation, we consider the case $B = 0$ (the finite B case is not more complicated in principle, but requires more work). In this case, the heat kernel is

$$P_0(\gamma) = 1 + \sum_{n=1}^{\infty}(2n + 1)e^{-\gamma(n^2+n)}, \tag{7.18}$$

measuring γ in units of $1/\epsilon_0$. Applying the Euler-Maclaurin summation formula to the sum in (7.18), we obtain the asymptotic expansion as $\gamma \to 0$

$$\begin{aligned} \sum_{n=1}^{\infty}(2n + 1)e^{-\gamma(n^2+n)} &\sim \int_0^{\infty} dn\ (2n + 1)e^{-\gamma(n^2+n)} - \frac{1}{2} - \frac{1}{12}(2 - \gamma) \\ &+ \frac{1}{720}(-12\gamma + 12\gamma^2 - \gamma^3) + \cdots = \frac{1}{\gamma} - \frac{2}{3} + \frac{\gamma}{15} - \cdots. \end{aligned} \tag{7.19}$$

We need to go to the third derivative term in the Euler-Maclaurin formula to obtain consistently the term proportional to γ (third is the lowest power of γ in the fifth derivative term).

As already mentioned the finite B calculation is similar, though somewhat more lengthy. The asymptotic behavior of the heat kernel is

$$P(\gamma) \sim \frac{1}{\epsilon_0 \gamma} + \frac{1}{3} + \frac{\epsilon_0 \gamma}{15} - \frac{g^2 \epsilon_0 \gamma}{6} - \cdots . \tag{7.20}$$

The important term in the asymptotic expansion (7.20) is the fourth one, proportional to γ and magnetic field dependent. It is easy to check that it can be rewritten in the form $-N_\Phi \hbar\omega\gamma/24$, hence it is manifestly equivalent to the corresponding term of the torus heat kernel. Therefore it will give rise to the same susceptibility as in the previous section - the Landau diamagnetism of the sphere and of the plane are identical.

7.4 The Landau diamagnetism of the hyperbolic plane.

To complete our study of constant curvature surfaces, we take up in this section the case of the hyperbolic plane - a surface with constant negative curvature. In three-dimensional Cartesian coordinates (x, y, z) it can be represented as the upper sheet ($z \geq R$) of the hyperbolic surface

$$-x^2 - y^2 + z^2 = R^2 .$$

The magnetic field B is everywhere orthogonal to the surface. We may call it the field of the hyperbolic monopole [75]. What is the magnetic response to the field of the hyperbolic monopole?

As before, we need the spectrum of the one-particle problem on the hyperbolic plane. It was determined by Comtet and Houston [77, 78] and was found to consist of two parts, discrete and continuous. Introducing the charge of the hyperbolic monopole $2g = 4\pi BR^2/\Phi_0$, in analogy with the case of the sphere, the discrete part of the spectrum was shown to be made of "Landau levels" $E_n = \epsilon_0(2gn + g - n - n^2)$, where n is a non-negative integer smaller than $g - 1/2$. Each Landau level is infinitely degenerate. The continuous spectrum is $E(\nu) = \epsilon_0(1/4 + g^2 + \nu^2)$, where ν is a positive continuous variable (the definition of ϵ_0 remains the same).

According to our scheme of calculating the magnetic part of the smooth thermodynamic potential, we need the heat kernel of the problem. Considering its definition, one immediately encounters the following problem. The heat kernel is the trace of the Green's function given by

$$G(\gamma, \mathbf{x}, \mathbf{x}') = \sum_{\{m\}} \psi_{\{m\}}(\mathbf{x}) \psi^*_{\{m\}}(\mathbf{x}') e^{-\gamma E_{\{m\}}}, \tag{7.21}$$

here by $\{m\}$ we mean the set of quantum numbers, which fully specifies the eigenstate; the sum should be understood as an integral when the quantum number is a

continuous variable. The trace involves the integration over the area of the hyperbolic plane, which is infinite, and strictly speaking the heat kernel diverges. What saves us is the fortunate circumstance that the Green's function (7.21) is independent of $(\mathbf{x}, \mathbf{x}')$, and therefore the area factors out of the trace (exactly what happens for the Euclidean space also). However we have now to calculate the wave functions as well to find the Green's function in (7.21). When this is done [77], the heat kernel can be worked out to be

$$\begin{aligned} P(\gamma) &= \frac{S}{4\pi R^2}\sum_{n=0}^{g-1}(2g-2n-1)e^{-\gamma\epsilon_0(2gn+g-n-n^2)} + \\ &\quad \frac{S}{2\pi R^2}\int_0^\infty d\nu\ \nu\tanh(\pi\nu)e^{-\gamma\epsilon_0(1/4+g^2+\nu^2)}, \end{aligned} \tag{7.22}$$

here we assumed for simplicity that g is an integer (the difference between this formula and the expression (3.6) in [77] can be understood taking into account the following identity, valid for integer g, $\mathrm{Im}(\Psi(1/2+i\nu-g)+\Psi(1/2+i\nu+g)) = \pi\tanh(\pi\nu)$, where Ψ is the logarithmic derivative of the Gamma function [8]); S is the area of the domain of the hyperbolic plane, defined by the location of the electron gas.

Now having the expression for the heat kernel at our disposal, we need its asymptotic behavior as $\gamma \to 0$. We start with the sum in (7.22). As in the previous section, the Euler-Maclaurin summation formula will do the job. The calculation is somewhat more involved than in the case of the sphere, because here the sum is finite. However as then, it suffices to go to the third derivative term in the Euler-Maclaurin formula in order to reach the γ-proportional part in the asymptotic expansion of the heat kernel. As a result we have

$$\sum_{n=0}^{g-1}(2g-2n-1)e^{-\gamma\epsilon_0(2gn+g-n-n^2)} \sim g^2 - \frac{\gamma\epsilon_0 g^2}{2} - \frac{\gamma\epsilon_0 g^4}{2} + \cdots. \tag{7.23}$$

As for the integral in (7.22), it is convenient to transform it using the identity $\tanh(\pi\nu) = 1 - \exp(-\pi\nu)/\cosh(\pi\nu)$. One of the resulting integrals is Gaussian and can be done exactly, another one, containing the hyperbolic cosine, is first developed in powers of γ, then each term in the series can be integrated, since it is of the form

$$\int_0^\infty dx\ \frac{x^{2m-1}e^{-x}}{\cosh x} = \frac{1-2^{1-2m}}{2m}|B_{2m}|\pi^{2m}. \tag{7.24}$$

Collecting the terms with the same powers of γ, we obtain

$$2\int_0^\infty d\nu\ \nu\tanh(\pi\nu)e^{-\gamma\epsilon_0(1/4+g^2+\nu^2)} \sim \frac{1}{\gamma\epsilon_0} - \frac{1}{3} - g^2 + \frac{\gamma\epsilon_0}{15} + \frac{\gamma\epsilon_0 g^2}{3} + \frac{\gamma\epsilon_0 g^4}{2} + \cdots. \tag{7.25}$$

The asymptotic expansion of the heat kernel for the hyperbolic plane is the sum of (7.23) and (7.25)

$$P(\gamma) \sim \frac{S}{4\pi R^2}\left(\frac{1}{\gamma\epsilon_0} - \frac{1}{3} + \frac{\gamma\epsilon_0}{15} - \frac{\gamma\epsilon_0 g^2}{6} + \cdots\right). \tag{7.26}$$

Again as it was for the sphere, the term responsible for the diamagnetism can be rewritten as $-N_\Phi \hbar\omega\gamma/24$, which would yield the magnetic susceptibility (7.9). Therefore we finally arrive at the conclusion that the smooth diamagnetic response (Landau diamagnetism) on all surfaces with constant curvature is the same.

The conjecture that comes in view of our result is that the Landau diamagnetic response is independent of the surface curvature. It seems that the most appropriate tools to consider this question are general heat equation methods [79]. Another open problem is to calculate the Pauli (spin) magnetic response on a general surface.

Chapter 8

Chiral boundary conditions for Quantum Hall systems.

8.1 Introduction.

In the previous chapters we considered finite-size systems, formulating the quantum-mechanical problem for them, which in mathematical nomenclature is called the boundary value problem. We did not devoted much thought to the choice of boundary conditions, assuming them to be Dirichlet. In this chapter we ask for a physical motivation for certain choice of boundary conditions. This is particular relevant for mesoscopic systems in the Quantum Hall regime, where right boundary conditions can naturally define bulk and edge of such system.

One of the main issues in Quantum Mesoscopic Physics is to study the behavior of many-particle quantum systems in confined geometries. For many purposes the many-body interactions are negligible and the problem reduces to that of one particle in a confined geometry. The corresponding Hamiltonian is a sum of a kinetic term and a one body operator describing either the confining potential or disorder in the bulk of the system. The expression "Quantum Mesoscopic Billiards" (QMB) was coined to describe generically this class of problems. The role played by the boundaries in the behavior of QMB is central. In the absence of bulk disorder, the shape of the boundary determines the nature of the energy spectrum, i.e. whether or not the system will show quantum signatures of chaos.

We begin by discussing in general terms what motivates the choice of a given set of boundary conditions and to see under which conditions this choice is justified for confined quantum systems in situations other than the QMB defined above, for instance for a many-body system when the Hamiltonian is not anymore quadratic or in the presence of a high magnetic field i.e. in the Quantum Hall regime.

8.1.1 How to choose boundary conditions?

Consider the case of a QMB without bulk disorder. It is described by the Hamiltonian $H = -\frac{\hbar^2}{2m}\Delta + V(r)$ where $V(r)$ is a confining potential. It is built up microscopically from the electrostatic description of two electron gases of different

dielectric characteristics. For a given ratio of the dielectric constants, the effective image force is strong enough to keep the electrons localized in a given area (the billiard). To know exactly the shape of the potential $V(r)$ and to solve for it the Shrödinger equation is a hopeless task. Then, under the assumption that $V(r)$ has bound states, it is possible to replace this problem by a simpler one, supposedly equivalent, defined by $H = -\frac{\hbar^2}{2m}\Delta$ and $\psi|_{\mathcal{B}} = 0$ for the wavefunction, where the boundary $\mathcal{B}$ is obtained from the symmetry and the shape of $V(r)$. This is the so called Dirichlet choice and it is widely used to describe QMB. A more technical remark is perhaps appropriate at this stage. This kind of "box quantization" obtained using Dirichlet boundary conditions is also widely used to describe other physical situations like, for instance, transport in a quantum system.

Although the Dirichlet choice is the most popular for the reasons discussed above, it is not the only one and may even lead to unpleasant surprises. Consider for instance the case of a confined Dirac particle (a Dirac billiard) described by:

$$\begin{pmatrix} 0 & D^\dagger \\ D & 0 \end{pmatrix} \begin{pmatrix} u \\ v \end{pmatrix} = E \begin{pmatrix} u \\ v \end{pmatrix}$$

instead of a Schrödinger Hamiltonian. Here, D and $D^\dagger$ are first order differential operators (the root of the Laplacian) and the wavefunction $\psi = \begin{pmatrix} u \\ v \end{pmatrix}$ is a two-component spinor. By demanding Dirichlet boundary conditions, the problem is over-determined and ψ is identically zero not only on the boundary but in the whole system. It is also known for this problem that other choices of local boundary conditions (e.g. Neumann) lead to difficulties associated with the creation of particle-hole pairs (Klein paradox) [80]. This problem is not only an academic curiosity, but might be relevant if one wants to describe mesoscopic superconducting billiards where the spectrum is obtained from the Bogoliubov-de Gennes Hamiltonian which, when linearized, belongs to the class of Dirac problems.

8.1.2 Beyond one particle: effective Hamiltonians.

So far we did consider the case of quadratic Hamiltonians i.e. the Laplacian plus a (one body) confining potential. When many-body effects cannot be neglected anymore, the situation is far more complicated. A standard form for the (tight binding) Hamiltonian is

$$H = \sum_i \epsilon_i c_i^\dagger c_i + \frac{1}{2}\sum_{ijkl} \langle ik|V|jl\rangle c_i^\dagger c_k^\dagger c_l c_j.$$

The kinetic part is still given (in a second quantized form) by a sum of Laplacian operators, but the second part associated with the interaction is a quartic term. Except for some special cases we do not know how to diagonalize such Hamiltonians no matter whether the system is bounded or not. The main issue underlying the search of various approximations is precisely to define instead an effective quadratic Hamiltonian whose parameters depend on the approximation. The well known perturbative or variational methods (Hartree Fock, RPA, Bogoliubov...) do fulfill this

objective. When dealing with confined many-body systems, we need to build an effective quadratic Hamiltonian whose potential takes into account both the many-body effects of the confined electrons but also, just like before, the effects of the electrostatic potentials resulting from the interactions with the surrounding environment.

Our choice of boundary conditions for the effective one body (quadratic) Hamiltonian is now broader and depends on the nature of the confining potential. If it is due to image forces as for the QMB case, then the Dirichlet choice will be again justified. But if the confinement is dominated by the many-body effects in the system itself, then we might be led to other choices of boundary conditions.

For the benefit of the more pragmatically inclined reader, let us illustrate these ideas by the example of the Feynman ansatz for N interacting bosons [81]. The many-body Hamiltonian is

$$H = E_0 - \frac{\hbar^2}{2m}\sum_i \Delta_i + V,$$

where $V = \sum_{i,j} V(|r_i - r_j|)$ is the interaction potential and E_0 the ground state energy. The N bosons wavefunctions describing the excited states is assumed (Feynman ansatz) to be of the form $\Psi(r_1, ..., r_N) = F\Psi_0(r_1, ..., r_N)$, where $F = \sum_i^N f(r_i)$ and Ψ_0 is the exact (but unknown) ground state wavefunction. This form is exact for the non interacting case, but it assumes for the interacting one that the interactions build up separately (under an adiabatic switching) in F and in Ψ_0. This approximation may be shown to be equivalent (under certain conditions) to the RPA, the generator coordinate method [82] or the quasi boson approximation. The equation of motion of the complex function $f(r)$ (it is not the wavefunction) is obtained by minimizing the energy $E = \frac{\langle\Psi|H|\Psi\rangle}{\langle\Psi|\Psi\rangle}$. Under the assumption of an incompressible ground state of density n_0, $\delta E = 0$ implies

$$-\frac{\hbar^2}{2m} n_0 \nabla^2 f = E \int d\mathbf{r}' f(r') n(r - r'),$$

where $n(r - r')$ is the density correlation function in the ground state Ψ_0. The effective energy E is now given by the quadratic form

$$E = -n_0 \frac{\hbar^2}{2m} \int d\mathbf{r} f^* (\nabla^2 f)$$

and to obtain the spectrum, we have to impose boundary conditions on the function f. Assuming translational invariance, Feynman obtained the well known relation $E = \frac{\hbar^2}{2m}\frac{k^2}{S(k)}$, where $S(k)$ is the structure factor. This gives the one branch phonon spectrum for small k. For a bounded system, relating $f(r)$ to the order parameter, we obtain that the fluid velocity is $\mathbf{v}(r) = \frac{1}{m}\nabla f$ so that the natural boundary conditions are Neumann, $\mathbf{n} \cdot \nabla f|_B = 0$ where $\mathbf{n}$ is a unit vector normal to the boundary. The same kind of approach applies to the case of bounded superconductors where the natural boundary conditions for the effective quadratic Hamiltonian are now generalized to [83]

$$\mathbf{n} \cdot (-i\hbar\nabla - \frac{2e}{c}\mathbf{A})|_B = i\lambda f$$

where λ is finite for the boundary between a superconductor and a normal metal while it is zero for an insulator.

To conclude, it looks to be quite a general result that where the Dirichlet boundary conditions are more appropriate for the case of a QMB (i.e. usual quantum mechanics), the Neumann (or elastic) boundary conditions appear to be the natural choice for collective (bosonic) excitations (phonons, plasmons...) which do appear in the effective quadratic approximations of many-body Hamiltonian. This is intimately related to the semi-classical nature of these approximations. They enable us, starting with the microscopic description, to reduce the problem to the study of large-scale modes for which boundary conditions should be formulated, according to macroscopic principles (like continuity of the current). This leads usually to Neumann boundary conditions.

8.1.3 Bounded Quantum Hall systems.

We go over to the application of the previous general remarks to the specific case of bounded electrons in a strong magnetic field i.e. in the Quantum Hall regime. We shall focus on the simpler case of non interacting electrons.

The various descriptions of the QHE's developed so far belong to two main categories. One is based on a bulk description, i.e. on the properties of a Landau like spectrum whose main characteristics are the large degeneracy of the ground state (proportional to the surface of the system) and its incompressibility, i.e. the existence of a gap between it and the first excited state. These conditions are enough to observe the quantization of the Hall conductance [84]. The surprising stability of these properties with respect to both disorder and interactions are partly responsible for the richness of this problem. Various points of view were developed in order to prove the quantization of the Hall conductance and among them a successful and promising topological approach [85, 86]. There, using periodic boundary conditions, the system has the topology of a torus so that edge physics does not play any role.

A second line of thought emphasizes the central role played by the edges. It is based on the idea that a magnetic field dependent incompressibility always leads to gapless edge excitations. Then, the total current being zero in the bulk (but not the current density), the currents in a Hall experiment flow along the edges [84, 87].

More recently, these edge states were presented as a possible realization of a quasi-one dimensional chiral electron gas. Various phenomenological models were developed to describe it, including a chiral Luttinger liquid [88, 89]. A global description which would relate these two approaches would be welcome. A microscopic way based on first principles to handle this question is difficult. To know the exact spectrum of the system, we first need to solve a classical electrodynamic problem to obtain the confining potential between two electron gases of different dielectric functions in a strong and inhomogeneous magnetic field. In the absence of applied magnetic field, the bulk excitations are plasmons with a dispersion $\omega \propto \sqrt{k}$. In the presence of the magnetic field the bulk spectrum acquires a gap (Kohn's theorem) equal to the cyclotron frequency and chiral edge magnetoplasmons propagating along the boundary do appear with a linear dispersion. Various descriptions were

proposed to study these edge excitations using different density profiles [90, 91]. Although these approaches do provide a qualitative description of the experimental results [92], they do not take into account quantum effects related to the quantization of the Hall conductance, a point which seems to be important experimentally [92].

It would be interesting to know if the microscopic confining potential could be replaced by an appropriate choice of boundary conditions which contain the same physics. To go further, we first consider the case of an effective one particle Hamiltonian of the form

$$H = -\frac{\hbar^2}{2m}(\nabla - \frac{ie}{\hbar c}\mathbf{A})^2 + V(r, \mathbf{B}),$$

where $\mathbf{B} = \nabla \times \mathbf{A}$ is the inhomogeneous magnetic field and $V(r, \mathbf{B})$ the effective confining potential, solution of the microscopic electrodynamic problem. To replace $V(r, \mathbf{B})$ by a set of boundary conditions, we have two main possibilities. The first one is to assume that it results from the electrostatics interactions and depends very little on the external magnetic field. This situation is similar to the QMB we discussed earlier and then we shall choose Dirichlet boundary conditions $\psi|_B = 0$. If on the other hand, the confining nature of the magnetic field plays a role, which is expected at high magnetic fields, then the Dirichlet choice might be non correct in the sense that although it confines the electrons, it will not be able to reproduce the edge excitations.

We are therefore looking for boundary conditions which connect together the bulk and edge properties of a confined Quantum Hall system. In other words, is there for this problem a generalized Poisson principle for which like in electrostatics, the bulk and edge excitations are a consequence one of the other?

These general considerations are presented in a more complete form in [93].

8.2 Boundary conditions for bulk and edge states in Quantum Hall systems.

We consider in this section the spectral properties of the magnetic QMB, stressing that along with the usual local boundary conditions, there is a place for the non-local boundary conditions in the theory of QHE. These, at first sight purely mathematical, constructs have a very appealing physical content by providing clear-cut edge and bulk notions for the Quantum Hall systems.

8.2.1 Motion in the absence of boundaries.

We consider first the problem of non interacting electrons without disorder moving in two dimensions in a uniform magnetic field B. The Hamiltonian can be expressed in terms of the two conjugate, first order differential operators D and $D^\dagger$ defined by

$$D = e^{i\theta}(\frac{\partial}{\partial r} + \frac{i}{r}\frac{\partial}{\partial \theta} + \frac{br}{2}) \tag{8.1}$$

and

$$D^\dagger = e^{-i\theta}(-\frac{\partial}{\partial r} + \frac{i}{r}\frac{\partial}{\partial \theta} + \frac{br}{2}) \tag{8.2}$$

as $\frac{2m}{\hbar^2}H = DD^\dagger - b = D^\dagger D + b$, where $b \equiv \frac{eB}{\hbar c}$ and the commutator $[D, D^\dagger] = 2b$. The spectrum of H for the infinite plane limit is

$$E_{nl} = \hbar\omega_c(n + \frac{|l| - l + 1}{2}), \tag{8.3}$$

where $l \in \mathbb{Z}$ is the angular quantum number, $n \in \mathbb{N}$ and $\omega_c = \frac{eB}{mc}$ is the cyclotron frequency. The ground state is obtained for $n = l = 0$ and its degeneracy is given by the total magnetic flux. This can be cast in the more general result which states that the Index defined by:

$$\text{Index} = \text{dim}\text{Ker}D - \text{dim}\text{Ker}D^\dagger \tag{8.4}$$

is equal to the degeneracy of the ground state [79, 94]. Ker$D$ (resp. Ker$D^\dagger$) defines the zero-modes of D (resp.$D^\dagger$), i.e. such that $D\Psi = 0$ (resp. $D^\dagger\Psi = 0$) and dimKer$D$ is the number of such independent solutions (resp. dimKer$D^\dagger$). For the problem at hand, this result is straightforward. For $B > 0$, Ker$D^\dagger$ is empty since $D^\dagger\Psi = 0$ implies $DD^\dagger\Psi = (2H + \hbar\omega_c)\Psi = 0$. Since the spectrum of H is non-negative, there is no non-zero solution. On the other hand, $D\Psi = 0$ implies $D^\dagger D\Psi = (2H - \hbar\omega_c)\Psi = 0$, which admits as a solution the lowest Landau level of energy $\frac{1}{2}\hbar\omega_c$. The Index is therefore infinite, as expected, but can be regularized noticing that except for the zero modes, $DD^\dagger$ and $D^\dagger D$ have the same spectrum. Then, since Ker$D$ = Ker$D^\dagger D$ and Ker$D^\dagger$ = Ker$DD^\dagger$, the Index in (8.4) is Index = $\lim_{t\to 0}\text{Tr}(e^{-tD^\dagger D} - e^{-tDD^\dagger})$. Expanding for small t we obtain:

$$\text{Index} = \frac{1}{2\pi}\int_{\mathbf{R}^2} d^2x[D, D^\dagger] = \frac{BS}{\Phi_0} \tag{8.5}$$

i.e. the degeneracy of the lowest Landau level. This result has been extended by Aharonov and Casher [95] to the situation of a spin half electron (Pauli Hamiltonian) in the plane submitted to a magnetic field of finite magnetic flux Φ. Since, in that case, the spectra of the Schrödinger and Pauli Hamiltonians are simply shifted by a constant $\frac{b}{2}$, their result can be immediately extended to the Schrödinger case. The ground state of energy $\frac{1}{2}\hbar\omega_c$ has a degeneracy given by Index = $[\Phi]$, where $[\Phi]$ is the integer part of Φ. These two examples are realizations of the Atiyah-Singer index theorem [79].

8.2.2 The Dirichlet boundary conditions.

So far, we have considered the case of open systems, i.e. with boundary conditions at infinity. Let us now return to the problem of electrons constrained to move in a disc of radius R in a uniform magnetic field (recall the semi-classical analysis of this system in the fifth chapter). The spectrum of this system has been studied and

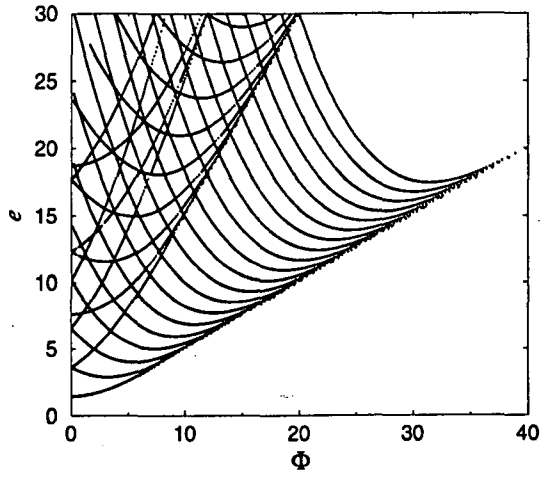

Figure 8.1: Spectrum of an electron in the magnetic field - Dirichlet boundary conditions. The energy e is plotted against the magnetic flux through the billiard Φ.

we recall some of the results. The angular momentum l is a good quantum number and the general solution of the Schrödinger equation is given by

$$\Psi_l(r) = Cr^{|l|}e^{-\frac{br^2}{4}}{}_1F_1(a, |l|+1, \frac{br^2}{2}), \tag{8.6}$$

where $a = \frac{|l|-l+1}{2} - \frac{\epsilon}{b}, \epsilon = \frac{2mE}{\hbar^2}$ and ${}_1F_1(a,c,x)$ is the confluent hypergeometric function. We first study the spectrum obtained by imposing local boundary conditions. For the sake of simplicity, we consider Dirichlet boundary conditions (DBC) i.e $\Psi_l(r = R) = 0$. The energy spectrum is then obtained from the zeros of ${}_1F_1(a, |l|+1, \Phi)$ which have been studied in detail. We can separate these zeros into two classes according to the sign of the angular momentum l. For $l \geq 0$, the corresponding energy levels are given by ${}_1F_1(\frac{1}{2} - \frac{e}{\Phi}, l+1, \Phi) = 0$ where $e \equiv \frac{2mR^2}{\hbar^2}E$ and $\Phi = bR^2 = \frac{BS}{\Phi_0}$ is the total magnetic flux through the disc in units of the flux quantum Φ_0. For $l < 0$, the energy levels are given by ${}_1F_1(-l+\frac{1}{2} - \frac{e}{\Phi}, |l|+1, \Phi) = 0$. The equation ${}_1F_1(a,c,x) = 0$ has solutions only for $a < 0$ and in the interval $-p < a < -p+1$, it has exactly p real solutions [96]. For instance, for $-1 < \frac{1}{2} - \frac{e}{\Phi} < 0$, there is one solution for each positive l. In the same interval, $-l + \frac{1}{2} - \frac{e}{\Phi} \geq 0$, so that there is no root in this interval for $l < 0$. Notice that the energy $\frac{e}{\Phi} = \frac{1}{2}$ which corresponds to the lowest Landau level is not an allowed solution for the disc with DBC (Fig. 8.1).

For any finite but large magnetic flux ($\Phi \gg 1$), the ground state is non degenerate, except in the limit $\Phi \to \infty$ where the degeneracy is infinite. Therefore, the conditions to display Quantum Hall Effect [84] are met only qualitatively under DBC. There are also other more formal problems with DBC. The degeneracy of the ground state is given by the Index which for the infinite plane limit is, the

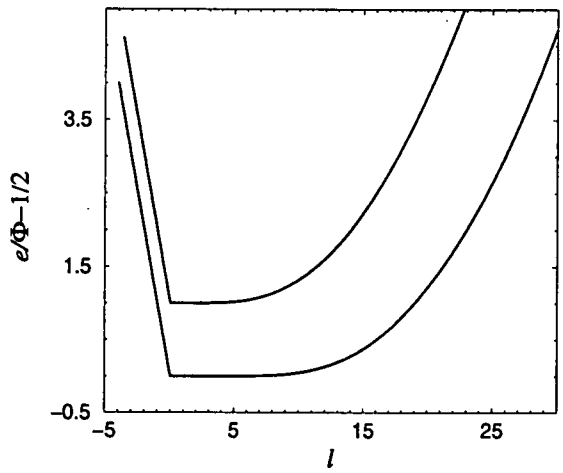

Figure 8.2: Spectrum of an electron in the magnetic field - Dirichlet boundary conditions. The energy $e/\Phi - 1/2$ is plotted against the angular momentum l. The total flux through the billiard is $\Phi = 20$.

total magnetic flux. With DBC, the Index is identically zero for any finite magnetic flux and becomes infinite for $\Phi \to \infty$. If we view our disc as embedded in the two-dimensional infinite plane with a magnetic field restricted to the area of the disc, then there is a contradiction with the Aharonov-Casher result. There is a continuity property of the Index as Φ is varied, based on Eq.(8.5) which should give at any Φ a non zero value. Moreover, the DBC lead to an ill defined problem for the calculation of the Index. The null spaces Ker$D$ and Ker$D^\dagger$ are obtained by solving the first order differential equations $D\Psi = 0$ and $D^\dagger\Psi = 0$. The general solutions of these equations are always strictly positive and cannot be identically zero on a finite domain. Therefore, they are incompatible with DBC. This problem has long been recognized by the mathematicians [97]. They were not motivated by those physical constraints, but by elliptic boundary value problems, i.e by the ellipticity of linear partial differential operators just like D and $D^\dagger$. The ellipticity of an operator on a manifold without boundary is equivalent to the invertibility of its symbol defined as the Fourier transform of the operator with respect to the momentum. This condition is fulfilled by D and $D^\dagger$. But if the symbol has a nonzero winding number, which happens when $[D, D^\dagger] \neq 0$, then ellipticity is incompatible with any local type of boundary conditions.

We summarize again the main features of the spectrum under the DBC (these features are more general though we demonstrated them only for the disc-like billiard). The lowest Landau level is always below the ground state ($l = 0$), although exponentially close. For any finite R, the ground state is non-degenerate. Since E_l are analytic functions of l (described as a continuous variable), there is no natural splitting in this spectrum between bulk and edge states (see Figure 8.2).

8.2.3 The Atiyah-Patodi-Singer boundary conditions.

There is another set of boundary conditions [97, 98] more adapted to this problem. We define the operator

$$J(r) \equiv \frac{i}{r}\frac{\partial}{\partial\theta} + \frac{br}{2}, \tag{8.7}$$

such that $D = e^{i\theta}(\frac{\partial}{\partial r} + J(r))$, as a generalized angular momentum. By projecting J on the boundary (circle of radius R), the corresponding spectrum is $\lambda(R) = -\frac{1}{R}(l - \Phi)$. It has both a positive and a negative part. The positive part contains all the l states corresponding to wavefunctions localized inside a radius R while for $\lambda \leq 0$, it gives those states localized outside this radius. Instead of local boundary conditions of the Dirichlet type, we might then consider the following non-local, Atiyah-Patodi-Singer (APS) boundary conditions [98]:

$$\Psi_l(R) = 0 \quad \text{for } \lambda \leq 0 \text{ i.e. } 0 < \Phi \leq l, \tag{8.8}$$

$$D\Psi_l|_{r=R} = 0 \qquad \text{for } \lambda > 0 \text{ i.e. } l < \Phi. \tag{8.9}$$

For wavefunctions localized outside the disc, we use as before the DBC (these are edge states), but for $l < \Phi$ i.e. for wavefunctions localized inside the disc, we impose mixed boundary conditions (this is the bulk). Therefore by construction we define two orthogonal parts of the full Hilbert space, which we call the edge and the bulk. What is the physical intuition behind such a splitting? As discussed already in relation with the semi-classical study of the energy spectrum in the fifth chapter, the Dirichlet boundary conditions do not provide a sharp dichotomy between bulk and edge states even for idealized situations. It is on the other hand a noticeable fact that such a dichotomy naturally exists for a classical bounded system in a magnetic field: for a given direction of the field, orbits that lie in the interior of the billiard rotate one way, while those hitting the edge make a skipping orbit and rotate in the opposite direction. Bulk and edge states are thus distinguished by their chirality relative to the boundary.

We return to the spectral properties of the APS problem. The APS boundary conditions are equivalent to DBC when $B = 0$. The solutions with DBC are $J_{|l|}(kR) = 0$ and the APS rewrites: $\Psi_l(R) = 0$ for $l \geq 0$ and $D\Psi_l|_{r=R} = 0$ for $l < 0$. But $D\Psi_l|_{r=R} = J_{|l|-1}(kR) = 0$ for $l < 0$. The APS and DBC spectra are therefore identical except for the degeneracy of the $l = 0$ state.

To compare the energy spectra obtained with each kind of boundary conditions, we first notice that the APS spectrum is obtained from the zeros of the same confluent hypergeometric function ${}_1F_1(a, c, x)$ as the DBC spectrum. This point is important and not obvious regarding the mixed boundary condition for $l < \Phi$.

i. For $0 < \Phi \leq l$, the boundary conditions are the same which gives:

$$e_l^S = e_l^D, \tag{8.10}$$

where e_l^S (resp. e_l^D) are energy levels for APS (resp. DBC).

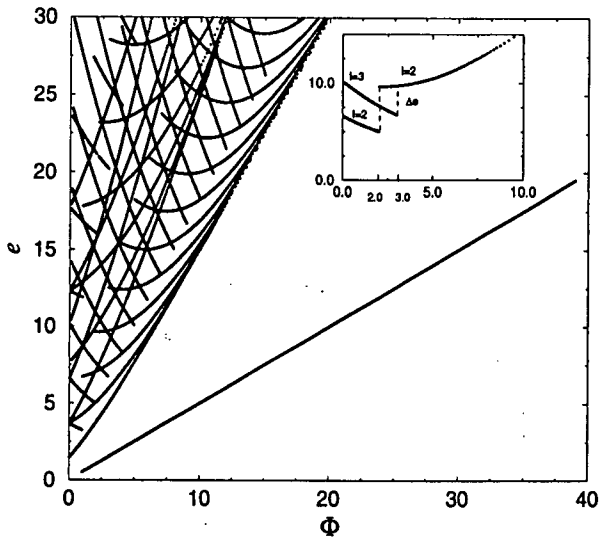

Figure 8.3: Spectrum of an electron in the magnetic field - APS boundary conditions. The energy e is plotted against the magnetic flux through the billiard Φ. The inset illustrates the discontinuity of the energy level $l = 2$, which occurs when $\Phi = 2$.

ii. For $\lambda > 0$ i.e. $l < \Phi$, there are two possibilities. For $l < 0$, $D\Psi_l|_{r=R} = 0$ gives ${}_1F_1(a, |l|, \frac{bR^2}{2}) = 0$ with $a = -l + \frac{1}{2} - \frac{e}{\Phi}$. Therefore this part of the energy spectrum corresponds to DBC and the exact connection with the DBC energies for $l < 0$ is given by:

$$e_l^S = e_{l+1}^D + \Phi. \tag{8.11}$$

Secondly, for $0 \leq l < [\Phi]$ the APS give $a_1F_1(a+1, |l|+2, \Phi) = 0$ [96] with $a = \frac{1}{2} - \frac{e}{\Phi}$ since $l \geq 0$. This equation has two sets of solutions. First, ${}_1F_1(a+1, |l|+2, \Phi) = 0$ for $a+1 < 0$ gives again Eq. (8.11). Second, $a = 0$, i.e.

$$e_l^S = \frac{\Phi}{2}. \tag{8.12}$$

For this value, ${}_1F_1(a+1, |l|+2, \Phi) \neq 0$ since $a+1 > 0$. Then, unlike for DBC, the lowest Landau level is now an allowed solution. Moreover, it has a finite degeneracy given by $[\Phi]$ since there is such a solution for each l between 0 and $[\Phi] - 1$. One could check, as might be anticipated, that these solutions define precisely the null space Ker$D$ (Ker$D^\dagger$ is empty for $\Phi > 0$ since the spectrum of H is non negative). Ker$D$ contains the solutions of $D\Psi_l(r) = 0$. With APS, this equation has a solution only for $0 \leq l < [\Phi]$, which is $a = 0$ (i.e $\frac{e}{\Phi} = \frac{1}{2}$) since ${}_1F_1(\frac{3}{2} - \frac{e}{\Phi}, |l|+2, \Phi) \neq 0$ for $a = 0$.

Let us summarize the main features of the APS energy spectrum. The ground state is given by the lowest Landau level ($e = \frac{1}{2}\Phi$) and it has a finite degeneracy given by the integer part of the enclosed magnetic flux.

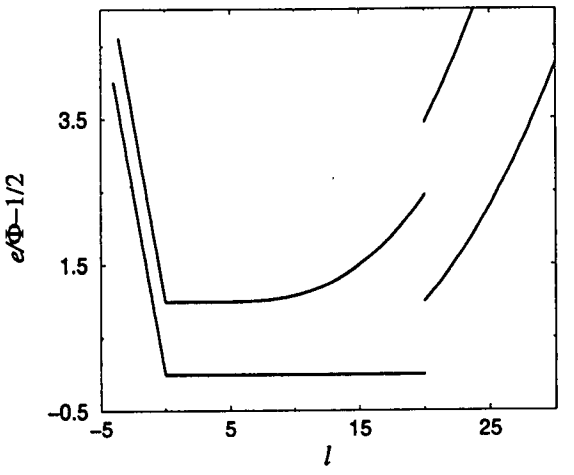

Figure 8.4: Spectrum of an electron in the magnetic field - APS boundary conditions (notations - as previously).

This ground state (the bulk) is separated from the first excited edge states by a gap equal to the cyclotron energy $\hbar\omega_c$. For $l \geq [\Phi]$, $e_l^D > \frac{3}{2}\Phi$ (property of the Dirichlet spectrum), and using Eq. (8.10) $e_l^S > \frac{3}{2}\Phi$. For $l < [\Phi]$, $e_l^D > \frac{1}{2}\Phi$ (general property of the Dirichlet spectrum), and according to (8.11) $e_l^S > \frac{3}{2}\Phi$ again. The energies of the excited states of the APS spectrum lie higher than $\frac{3}{2}\hbar\omega_c$ thus forming a gap with the ground state.

We emphasize again that the energies e_l^S (for fixed l) are not continuous functions of the magnetic flux Φ. For fluxes $0 < \Phi \leq l$, we have $e_l^S = e_l^D$. But for $\Phi > l$, the boundary conditions change and a discontinuity occurs: $e_l^S = e_{l+1}^D + \Phi$. For $l-1 < \Phi < l$, we have $e_{l+1}^S = e_{l+1}^D$ and therefore, the two states of angular momentum $l+1$ and l are separated in energy by $\hbar\omega_c$ (Fig. 8.3).

The APS and DBC spectra do present different characteristics (compare Figures 8.2 with 8.4). The APS spectrum has an incompressible degenerate ground state separated from the first excited states by a gap equal to $\hbar\omega_c$, i.e. independent of the size of the system. This result cannot be obtained perturbatively from the weak field ($\Phi \to 0$) limit since for $\Phi < 1([\Phi] = 0)$ we recover the Dirichlet spectrum. Moreover, the ground state energy ($e = \frac{1}{2}\Phi$) does not depend on the angular momentum l so that it does not carry any current in the presence of an external magnetic flux. Most importantly however the APS description offers a natural definition of the edge versus bulk in the Hibert space of the problem.

8.2.4 The chiral boundary conditions.

The discontinuity in the APS spectrum is undesirable for Quantum Hall systems, invalidating considerations based on adiabatic evolution with an external parameter.

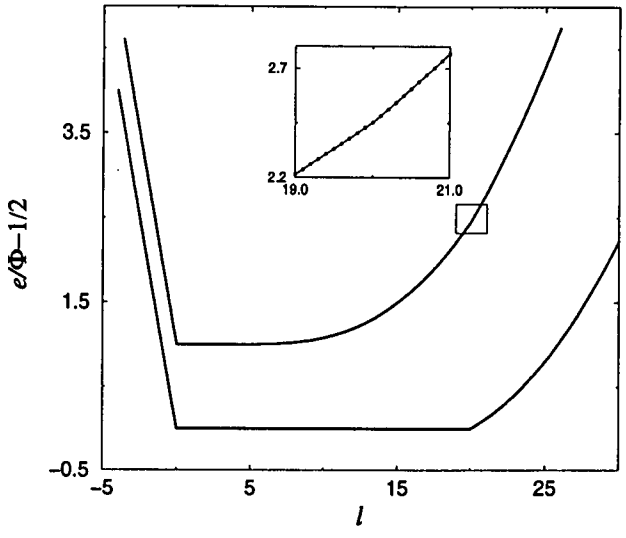

Figure 8.5: Spectrum of an electron in the magnetic field - chiral boundary conditions (inset - enlarged box, showing a cusp between bulk and edge states; notations - as previously).

We can avoid it defining the Chiral Boundary Conditions (CBC), which are close relatives of the APS and therefore preserves the edge versus bulk dichotomy of the Hilbert space. The chiral boundary conditions require:

$$\begin{aligned} D\psi_l(r)\Big|_{r=R} &= 0, \quad \text{for } \lambda \leq 0 \ , \\ \partial_r\psi_l(r)\Big|_{r=R} &= 0, \quad \text{for } \lambda > 0 \ . \end{aligned} \tag{8.13}$$

The first condition (8.13), corresponding to the bulk, remains unchanged. In contrast with the APS problem, the second condition (8.13) requires the zero normal derivative (Neumann boundary conditions) for the edge. It can be checked directly that this choice preserves gauge invariance and defines a self-adjoint eigenvalue problem (these questions are discussed in the Appendix, where the CBC are formulated and applied for the case of the semi-infinite cylinder).

The energy spectrum can be described in terms of special functions as in the previous cases and is shown on Fig.8.5. The edge energies now join continuously the bulk, however the slope is discontinuous between them, reflecting the different boundary conditions we imposed on edge as opposed to bulk. The edge spectrum is gapless in the thermodynamic limit and has a linear dispersion for low excitation energies with a "sound velocity" proportional to $\sqrt{B}$. Another justification of Neumann boundary conditions for the edge states is this - the Dirichlet original choice of APS pushes away the edge states from the boundary.

8.3 The Hall conductance and the non-local boundary conditions.

In this section we would like to propose a new relation for the Hall conductance for the APS problem. Before starting to discuss the transport, we need to return to the calculation of the Index. There is a natural relation between the finite degeneracy of the ground state obtained with the APS boundary conditions and the Index. In fact the APS problem was considered in order to give a meaning to the Index theorem for the case of elliptic boundary problem on manifolds with boundaries. The demonstration of this general result, known as the Atiyah-Patodi-Singer theorem [98] is beautiful but far beyond the scope of our discussion. We shall simply show here how it works in our case.

First we notice that by definition, the Index should be an integer. This is clear for the Aharonov-Casher case, and also for the Index defined on a compact manifold without boundary like the sphere or the torus. It comes from the quantization of the magnetic field in these geometries. For the infinite plane, the index is infinite, but this can be viewed as a limiting case of the previous one. For the disc geometry or other manifolds with boundaries, the total flux through the system is not quantized and therefore Eq.(8.5) poses problem. The APS theorem states that there is a correction to the total magnetic flux because of the boundaries which can be expressed through the SBC (only) such that the Index theorem rewrites:

$$\text{Index} = \Phi - \frac{1}{2}(h + \eta(0)), \tag{8.14}$$

where h is the number of zero eigenvalues of $J(R)$; and $\eta(0)$ is defined by the difference between the positive and negative λ's:

$$\eta(0) = \sum_{\lambda(R)>0} 1 - \sum_{\lambda(R)\leq 0} 1. \tag{8.15}$$

Since the spectrum of $J(R)$ is infinite, $\eta(0)$ is ill-defined and needs to be regularized. This can be done using

$$\eta(0) = \lim_{s\to 0} \sum_{\lambda\neq 0} \text{sgn}(\lambda)|\lambda|^{-s}. \tag{8.16}$$

We shall now calculate explicitly the various quantities which do appear in Eq.(8.14) and show that in our case they do fulfill the APS theorem. Defining the integer [...] and fractional $< ... >$ parts of a given number, we write

$$\lambda(R) = -\frac{1}{R}(l - \Phi) = -\frac{1}{R}(l - [\Phi] - < \Phi >),$$

where $0 \leq < \Phi > < 1$. We assume for the sake of simplicity that $< \Phi > \neq 0$. Then, $\lambda(R) \neq 0$ and $h = 0$. Defining the integer $p = l - [\Phi]$, we can rewrite

$$R^s \eta(s) = \zeta(s, 1 - < \Phi >) - \zeta(s, < \Phi >),$$

where

$$\zeta(s,x) \equiv \sum_{p=0}^{\infty}(p+x)^{-s}$$

with $x > 0$. The function $\zeta(s,x)$ is analytic in $s = 0$ and $\zeta(s=0,x) = \frac{1}{2} - x$. This gives $\eta(0) = -1 + 2 < \Phi >$ and

$$-\frac{1}{2}(h + \eta(0)) = \frac{1}{2} - < \Phi > . \tag{8.17}$$

This looks at odd with the expected result, Index $= [\Phi]$, because of the remaining factor $\frac{1}{2}$. But the divergence of $-\frac{l}{r} + \frac{br}{2}$ at the origin introduces there a new effective additional boundary where $\eta(r = 0, 0) = 0$ and $h(r = 0) = 1$ so that Index $= \Phi - <$ $\Phi >= [\Phi]$ as expected.

In order to study the Hall transport we need the current response to an applied voltage. There are two different lines of argument in order to obtain the Hall conductance. The first one based on the Laughlin-Halperin [99, 100] description, gives the current I as a response to a static AB flux. Since the edge states in the disc geometry do have a finite angular momentum, their energy levels are obtained by the replacement $l \to l + \phi$. The current of a given level $e(n, l + \phi)$ is

$$i(n,l) = \frac{\partial e(n, l+\phi)}{\partial l}, \tag{8.18}$$

and the total current, for a given chemical potential μ, is

$$I = \sum_{n,l} i(n,l)\theta(\mu - e(n,l)). \tag{8.19}$$

It is, in the mesoscopic terminology, a persistent current i.e. the thermodynamic response of the system to a static AB flux. The variation of I with μ defines the Hall conductance $\sigma_H = \frac{dI}{d\mu}|_B$. This approach has been extended by MacDonald [84] and is equivalent to the Widom-Středa formula.

In contrast, there is another picture for the Hall conductance based on topological quantum numbers, which uses also external AB [85, 86] fluxes. There, the system has the topology of a torus so that edge states are naturally absent. One of the external fluxes $\phi(t)$ is time-dependent and plays the role of a battery. The induced Hall current I_{ad} calculated within the adiabatic limit is $I_{ad} = I + \Omega\dot{\phi}$ where Ω is the adiabatic curvature and I the persistent current (discussed above) associated with the static part of ϕ. The adiabatic curvature is by construction a conductance and is equal to the Hall conductance derived from the Kubo formula [85, 86]. It is a topological invariant, namely a Chern number, obtained by averaging the adiabatic curvature over the torus phase space but this is not enough to guarantee their stability (as integers) with respect to disorder or interactions.

In order to get rid of the averages over the AB fluxes, Avron et al. [101] following Bellissard [102], defined an index of projection which can be understood in the example of the infinite plane as a measure of the charge transfer from the origin to infinity due to the change of a static AB flux. This index of projection has the same

physical content as the Laughlin-Halperin description. Moreover, for the infinite system, it coincides with the adiabatic curvature [94]. But for a finite size system, it is identically zero and its relation to the Hall conductance has not yet been put on a firm physical ground.

We would like to show that these various points of view which may look at odd, can be accommodated and even related in a quantitative description by using the non-local APS boundary conditions. The basic underlying mechanism for the transfer of charges is those given by the Laughlin-Halperin picture and can be understood as well using the DBC. But the APS do provide a natural way to relate the Hall conductance to the change of the function η associated to the boundaries and to the Index describing the degeneracy of the incompressible ground state.

Let us first discuss in more details the response to a AB flux ϕ piercing the disc at the origin. This could be understood as a change of boundary conditions where the disc is cut along a radial direction and $e^{2i\pi\phi}$ boundary conditions are imposed across the cut. Therefore the spectrum is ϕ-periodic with period one (in units of $\Phi_0 = \frac{hc}{e}$). Let us see how this works for the infinite plane. For $\phi = 0$, the energy level $n = 0$ contains only positive angular momenta $l \geq 0$ states, $n = 1$ contains in addition $l = -1$ and so forth. When ϕ changes from 0 to 1, the state $l = -1$ changes its energy from $\frac{3}{2}\hbar\omega_c$ to $\frac{1}{2}\hbar\omega_c$ and takes the place of the $l = 0$ state. This can be viewed as an overall transfer of charge within the lowest Landau level of an additional charge at the origin ($l = 0$) which migrates to infinity. This description which is easily generalized to the higher Landau levels underlies the definition of the projection index of Avron et al. [101] as the difference of occupied states in a given Landau level when ϕ varies from 0 to 1. This number is infinite in both cases but the difference is finite and equals one. This charge transfer between the "edges" through a Landau level is precisely those given by the Laughlin-Halperin picture. For a finite size disc we shall consider first the case of DBC and a chemical potential $\frac{1}{2}\hbar\omega_c < \mu < \frac{3}{2}\hbar\omega_c$ so that there are only states $l \leq 0$. For $\phi > 0$, the corresponding energy levels depend on $l + \phi$ and as ϕ is changed from 0 to 1, they move towards the outer radius of the disc. Consider now the state $l = -1$. Its energy along the direction $e = \frac{5}{2}\Phi$ is obtained from the Laguerre polynomial $L_1{}^{1-\phi}(\Phi) = 0$ and for $\phi = 1$, $e(l = -1, \phi = 1) = \frac{3}{2}$ and this level has the same energy that the state $l = 0$ for $\phi = 0$. The generalization of this calculation is straightforward and gives finally a picture of the charge transfer identical to those obtained for the infinite plane limit. The total current for a maximum angular momentum $L(\mu)$ corresponding to a given chemical potential $\mu < \frac{3}{2}\hbar\omega_c$ is

$$I = \sum_{l=0}^{L-1} \frac{\partial e}{\partial l}(l, n = 0). \tag{8.20}$$

For the low values of l, $\frac{\partial e}{\partial l} \simeq 0$ (Fig.1) and these are the bulk states, while for higher values of l (edge states), we may consider l as a continuous variable so that $I \simeq e(L) - e(1)$. The energy $e(L(\mu))$ is obtained by projecting this state at fixed energy onto the direction $e = \frac{3}{2}\Phi(\mu)$. Then,

$$\frac{dI}{d\mu}|_{\Phi} = \frac{3}{2}\frac{d\Phi(\mu)}{d\mu} = 1$$

since $\Phi(\mu) = \frac{2}{3}\mu$. This defines for $\mu < \frac{3}{2}\hbar\omega_c$, a Hall conductance $\sigma_H = 1$ in units of $\frac{e^2}{h}$. The generalization to higher energies gives $\sigma_H = n$ where $n \in \mathbb{N}$. But this calculation relies on the approximation obtained by replacing the angular momentum by a continuous variable and derivatives by differences. Moreover, this cannot be extended to disordered systems since l is not a good quantum number anymore. In that case we see that the projection index is identically zero since for a finite chemical potential μ, the number of gained states just compensates the lost states with final energies (for $\phi = 1$) larger than μ. We then propose the following scheme. We define the spectral flow $\Delta(\phi)$ due to an external flux ϕ as the change:

$$\Delta(\phi) = \frac{1}{2}(\eta(\phi) - \eta(0)), \tag{8.21}$$

where $\eta(\phi)$ is the extension of $\eta(0)$ defined by Eq.(8.15). Let us show now that the spectral flow measures precisely the transfer of charge between the two edges as described before [103]. The function η is defined from the spectrum of the operator J. For the case of an additional AB flux (for instance $\phi < 0$) at the origin, this spectrum is $\lambda_l(R, \phi) = -\frac{1}{R}(l - \phi - \Phi)$. The regularity of the wavefunction ($\propto r^{l-\phi}$) at the origin $r = 0$, imposes $l - \phi \geq 0$. In order to fulfill the new spectral boundary conditions, we need $\lambda_l(R, \phi) > 0$ i.e. $l < \phi + \Phi$. The Index is then given by $\text{Index}(\Phi, \phi) = [\Phi + \phi] - [\phi]$ and when ϕ changes from 0 to 1, there is one eigenvalue $\lambda_l(R)$ of J which changes sign, thus describing a state which jumps from the ground state ($e = \frac{1}{2}\Phi$) with $\lambda > 0$ to the first excited edge state with $\lambda \leq 0$. By definition $\Delta(1)$ measures this jump and $\Delta(1) = 1$, which can be checked directly from the definition Eq. (8.21). This mechanism, which can be generalized to higher states, is exactly that described qualitatively above for the case of DBC or for the infinite plane with the help of the index of projection. Then, we propose for the Hall conductance the relation:

$$\sigma_H = \frac{dI}{d\mu}|_\Phi = \Delta(1) \tag{8.22}$$

which relates σ_H to the overall spectral flow when the external flux ϕ varies from 0 to 1.

Let us emphasize again that, although the underlying mechanism for the charge transfer is not specific to the APS problem, but can be understood as well with DBC, for the latter case Index $\equiv 0$, while for APS it can be defined safely and σ_H can be related to the spectral flow Δ.

We would like now to extend this approach in order to include disorder. It does not generalize to any class of disorder potential, because of the assumption that we can define two operators D and $D^\dagger$ in such a way that the total Hamiltonian $H = DD^\dagger - V(r) = D^\dagger D + V(r)$. For instance, this might describe the case of a random magnetic field $B(r)$ with a constant flux through the disc. Or we could also consider modifying the shape of the boundary, which instead of a circle might be any smooth but random function of fixed length in order to conserve the total magnetic flux. We know from the study of ballistic billiards in mesoscopic physics, that weakly disordered metals share with ballistic chaotic billiards number of similarities, for instance energy spectra described by the Wigner-Dyson statistics

[104]. This qualitative relation between a bulk disorder and a modification of the boundary shape can be checked for instance by considering the case of an elliptic billiard [105]. There, at low magnetic field, the spectrum is well described by the Wigner-Dyson statistics and for higher fields, the directions corresponding to Landau levels are broadened while the edge states with "high angular momentum" look quite unaffected. These characteristics were already recognized and studied, but a quantitative description is still missing since the angular momentum l is not a good quantum number anymore.

The main result of this chapter is that particular choice of non-local boundary conditions can naturally define the bulk and edge of the Quantum Hall systems, by separating the total Hilbert space of the problem into two orthogonal sub-spaces. In the case of the Atiyah-Patodi-Singer boundary conditions some Index theorems hold, useful to calculate the Hall conductance. However the spectrum is discontinuous as a function of external parameters. The chiral boundary conditions remove the discontinuities, retaining the clean bulk and edge separation.

Chapter 9

Conclusion.

In this thesis we developed the point of view that the methods of asymptotic analysis can be successfully applied to the calculation of smooth thermodynamic quantities. The main conclusion is that dome of the other methods, currently in use, are less suited, or even unable to reach comparable achievements. Thus, we show that disorder averaging of the thermodynamic current (a quantity that in the Green's function formalism involves average over *one* Green's function) is equivalent to the asymptotic smoothing over the spectrum of a *clean* system, instead of dealing with the actual spectrum of the disordered system. However the properties of these two spectra are essentially different, therefore even intuitively we would expect that if the smooth quantities should coincide, this would happen only to the leading order of the asymptotic expansion. On the other hand, the supersymmetric technique of averaging over the disorder, when applied to evaluate disorder averages of quantities given by a single Green's function (for example the density of states), yields results that are equivalent to those obtained in the framework of Random Matrix theory. Yet by considering the magnetic response of mesoscopic systems (magnetization, persistent currents) within the RMT framework, we certainly miss the effects of the spectrum characteristics.

We summarize in a more specific way the main results of this thesis and point out some developments they may suggest. We follow the order of the chapters.

- The smooth persistent current in a clean ring is zero. This does not generalize to all disordered systems, as shown for instance by the Kronig-Penney model. It is important to understand what general properties of the spectrum cause the vanishing of the current, in other words how much information do we need about the spectrum to obtain the current. The study of the Scarf's model is a first step in that direction. This would help us to shed some light to the persistent current problem, which is a canonical problem in the description of thermodynamic properties of mesoscopic systems. In particular we hope to solve the many-channel ring case, which still seems to be the most interesting and relevant system experimentally.

- The smooth response to an Aharonov-Bohm vector potential (local gauge transformation) is non-zero, in contrast with the result obtained previously

for rings. This means quite interestingly that the properties regarding the magnetic response of the continuous spectrum differ from those of the discrete one. There is a straightforward but time-consuming thing to do - to continue the calculation of the magnetization, and to find at which order of the asymptotic expansion in large $k_F R$ the non-zero result is obtained. This is an interesting question, because in such an open system, the magnetization is not trivially related to the current. Probably the magnetization reflects other aspects of the magnetic response not contained in the current.

- The random walk asymptotic description of quantum localization was studied in order to prove its equivalence to the self-consistent diagrammatic method. This description should be generalized to systems in a magnetic field, since no conclusive results were obtained so far on the mobility edge in comparatively weak magnetic field (there are field-theoretical results in the Quantum Hall regime). Then, the relation to the classical Heisenberg model should be studied, since within this model there is a possibility to define and generalize the Thouless curvature, and probably extend its validity to obtain universal conductance fluctuations. Finally, our approach should be extended to include the dependence of the diffusion constant on the wavevector, for which the multifractal structure of the wavefunctions at the mobility edge can be probed. This may help to answer questions about the universality of "the gang of four" description of the localization transition for general spectra.

- We have shown how to calculate accurately the energy levels (including the lowest) of integrable magnetic billiards using a semi-classical approach. These powerful methods might be generalizable to the case of non-integrable (classically chaotic) systems.

- We have used the method of Stewartson and Waechter to generate the Weyl asymptotic series for the semi-infinite cylinder in a magnetic field. This method works as well for the disc. However Stewartson and Waechter have developed a more general approach to find recursively the terms in the heat kernel expansion, knowing just the curvature (and its derivatives) of the billiard. Could this method be generalized to the heat kernel expansion of general magnetic billiard? Another open question (considered in the recent work of Berry and Howls) is the relation between the asymptotic heat kernel expansions and the semi-classical methods like those used previously for the calculation of the spectrum of integrable systems. This is an interesting mathematical problem, since basically the shape of the two-dimensional system defines it completely (we can hear the shape of a two-dimensional singly-connected billiard).

- On the example of the Landau diamagnetism calculation we showed that a relation exists between the smoothing and finding the best approximation of a quantity using the least squares method. This connection deserves a further study. We also found that the smooth diamagnetic response is identical in the case of two-dimensional surfaces of constant curvature (plane, sphere

and hyperbolic plane). We conjecture that this result should generalize to any sufficiently smooth two-dimensional surface. We would like to examine a similar problem for the Pauli paramagnetism. Is the ratio between the Landau orbital diamagnetism and Pauli spin paramagnetism universal? What makes this problem interesting are the topological invariants that exist for the Pauli Hamiltonians.

- The main conclusion of this chapter is that although the Dirichlet boundary condition is a natural choice, it might not be always the best one from a physical point of view. Those cases pertain to interesting problems, which are now under current interest in condensed matter physics. One of them is the spectrum of a superconducting island in a normal substrate, when the Dirichlet boundary condition is inappropriate since it over-defines the problem. Another is the Hall liquid droplet (Fractional Hall regime). There, apparently normal to the boundary component of the current should vanish; in addition we should preserve the bulk-edge duality (crucial to the physics of the Quantum Hall Effect). The non-local boundary conditions we introduced and studied, are tailored exactly in order to fulfill those constraints. They contain both bulk and edge states with their corresponding physical properties - a degenerate ground state for the bulk and a gapless excitation spectrum for the edge. However we did not yet succeed to find a microscopic way, from which the chiral boundary conditions would be a naturally consequence.

Appendix

Boundary Conditions for Bulk and Edge States in Quantum Hall Systems

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Abstract. For two dimensional Schrödinger Hamiltonians we formulate boundary conditions that split the Hilbert space according to the chirality of the eigenstates on the boundary. With magnetic fields, and in particular, for Quantum Hall systems, this splitting corresponds to edge and bulk states. Applications to the integer and fractional Hall effect and some open problems are described.

Submitted to J. Phys. I France

The theory of the Quantum Hall Effect has been torn between several schools of thought: one stresses the two dimensional bulk aspects of the interior [1]; another emphasizes the importance of the one dimensionality of the edge [2] and other points of view focus on the interplay between bulk and edge [3]. It is therefore remarkable that in spite of this the notion of bulk and edge of a quantum system is not formulated as a sharp dichotomy even for idealized situations. Classically, there is such a dichotomy for billiards in magnetic fields: orbits that lie in the interior rotate one way, say clockwise, while orbits that hit the edge make a skipping orbit and rotate counter-clockwise [4]. Bulk and edge are therefore distinguished by the chirality relative to the boundary. Our purpose here is to formulate a corresponding dichotomy in quantum mechanics. As we shall explain this can be achieved by imposing certain *chiral* boundary conditions for Schrödinger and Pauli operators.

The chiral boundary condition we introduce is sensitive to the direction of the (tangential) velocity on the boundary. For (separable) quantum billiards this enables us to split the one particle Hilbert space into a direct sum of two orthogonal, *infinite dimensional* spaces with positive and negative chirality on the boundary. In the presence of a magnetic field, this split gives a Hilbert space for edge states, $\mathcal{H}_e$, and a Hilbert space for bulk states, $\mathcal{H}_b$, such that the full Hilbert space is $\mathcal{H} = \mathcal{H}_e \oplus \mathcal{H}_b$. Subsequently we shall explain how chiral boundary conditions are formulated for Schrödinger Hamiltonians which do not necessarily correspond to separable billiards, i.e. Schrödinger Hamiltonians with background potential and electron-electron interactions.

The chiral boundary condition we introduce is a relative of a boundary condition introduced by Atiyah, Patodi and Singer (APS) in their studies of Index theorems for Dirac operators with boundaries [5]. However, the chiral boundary condition we shall introduce differs from it in an important way, as we shall explain below.

The splitting of the Hilbert space comes with a splitting of the quantum billiard Hamiltonian and its spectrum to a bulk piece and an edge piece. As we shall see, it is a property of the chiral boundary conditions that the bulk spectrum has a ground state at precisely the energy of the lowest Landau level in the infinite plane, and a degeneracy which is the total flux through the billiard, (corrected to an integer number of flux units by a boundary term). The bulk energy spectrum has a gap above the ground state, which for separable billiards, is the gap between Landau levels in the infinite plane. This gap survives in the thermodynamic limit of a billiard of infinite area, the bulk ground state is guaranteed to be incompressible in this sense.

In contrast, the edge spectrum, in the thermodynamic limit of long boundary is gapless. In this limit, the edge states have a well defined "sound velocity", which reflects the linearity of the dispersion relation at low energies. The sound velocity v is

$$v/c = k\,(\hbar/mc)\,\sqrt{B/\Phi_0}, \tag{1}$$

where k is a dimensionless (nonuniversal) constant, c is the velocity of light , $\frac{\hbar}{mc}$ is the Compton wavelength of the electron and $\sqrt{\Phi_0/B}$ is the magnetic length. This velocity is very small in all reasonable magnetic fields.

The splitting of the Hilbert space enables us to describe charge transport in terms of spectral flow. In particular, (adiabatic) gauge transformations can transfer states between $\mathcal{H}_e$ and $\mathcal{H}_b$. For the semi-infinite cylinder, such a spectral flow is described below. This generalizes the Index theory of the Integer quantum Hall effect [6] to systems with boundaries.

We start with the semi-infinite cylinder for which we shall illustrate the chiral boundary condition. The Landau Hamiltonian with chiral boundary condition is separable and a complete spectral analysis can be made.

Consider the semi-infinite cylinder, M, in $\mathbb{R}^3$, whose boundary ∂M is a circle with a circumference ℓ: $M = \{(x,y) \mid -\infty \le x \le 0,\ 0 \le y < \ell\}$. The orientation of M and the orientation of the boundary, ∂M, are linked by requiring that traversing the boundary in the positive direction keeps M on the *left* hand side.

A constant magnetic field perpendicular to the surface, of strength $B > 0$ and with outward orientation acts on the surface. We take the charge of the electron to be positive (sic!) so classical (bulk) electrons in the interior of M rotate clockwise. In addition we assume that a flux tube carrying flux ϕ threads the cylinder. We shall regard ϕ as a parameter, while B is kept fixed throughout. A gauge field describing the situation is $A(\phi) = (0, Bx + \phi/\ell)$. The velocity operator, in units $m = \hbar = e/c = 1$, is $(v_x, v_y) = (-i\partial_x, -i\partial_y - Bx - \phi/\ell)$. The classical energy associated to a particle on a billiard is purely kinetic, $E = v^2/2$. The corresponding quantum Hamiltonian is the Landau Hamiltonian given formally by the second order partial differential operator:

$$2H_L(\phi) = D^\dagger(\phi)D(\phi) + B, \tag{2}$$

where $D(\phi) = iv_x - v_y(\phi, x) = \partial_x + (i\partial_y + Bx + \phi/\ell)$.

For this to define a self-adjoint operator in the one particle Hilbert space we need to specify boundary conditions on ∂M.

The chiral boundary condition that we introduce requires different things from the wave function on the boundary depending on the tangential velocity, $v_y(\phi, x)$ at the boundary $x = 0$. Since $v_y(\phi, 0) = -i\partial_y - \phi/\ell$ commutes with D we separate variables, and describe the chiral boundary conditions for the resulting ordinary differential operators on the half line $-\infty \le x \le 0$, parameterized by $m \in \mathbb{Z}$ and $\phi \in \mathbb{R}$:

$$2H_m(\phi) = -\frac{d^2}{dx^2} + \left(\frac{2\pi m - \phi}{\ell} - Bx\right)^2. \tag{3}$$

Let

$$D_m(\phi) = \frac{d}{dx} - \frac{2\pi m - \phi}{\ell} + Bx. \tag{4}$$

The chiral boundary condition requires:

$$\begin{aligned} D_m f_m\big|_{x=0} &= 0, \quad \text{if} \quad v_y(\phi,0) = \frac{2\pi m - \phi}{\ell} \le 0; \\ (iv_x)\, f_m\big|_{x=0} &= 0, \quad \text{if} \quad v_y(\phi,0) = \frac{2\pi m - \phi}{\ell} > 0. \end{aligned} \tag{5}$$

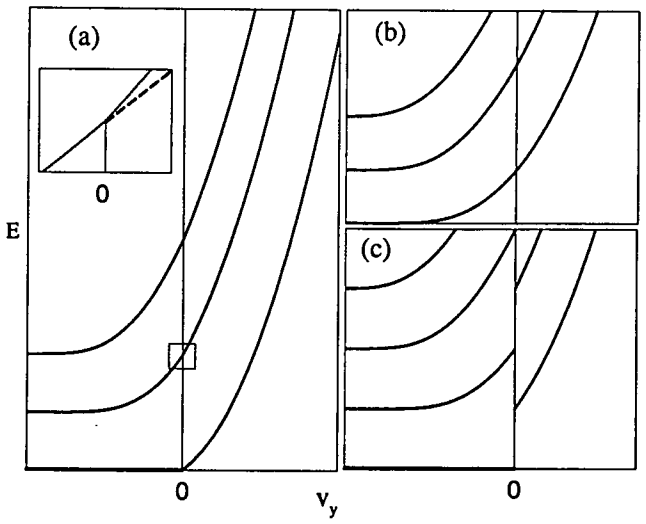

Figure 1: Spectrum of Landau Hamiltonians: (a) with chiral boundary conditions (inset - enlarged box, showing a cusp between bulk and edge states), (b) with Dirichlet boundary conditions, (c) with APS boundary conditions.

A classical electron in the bulk rotate clockwise, and so its velocity near the boundary *disagrees* with the orientation of the boundary. For such an electron we require *spectral* boundary conditions, $(D_m f)(0) = 0$, which are m-dependent elastic boundary conditions (an interpolation between Neumann and Dirichlet). A classical skipping orbit moves in a direction that agrees with the orientation of the boundary, and for positive velocity on the boundary we impose Neumann boundary condition. We shall say more on the reasons for choosing spectral and Neumann for the different chiralities below.

Since both the differential operator, and the boundary conditions are defined in terms of velocity, gauge invariance is manifest. Moreover, it can be checked that the boundary conditions in Eq. (5) define a self-adjoint eigenvalue problem, which we shall call the chiral Landau Hamiltonian. The spectrum and eigenfunctions can be described in terms of special functions [7].

The bulk space $\mathcal{H}_b$ is defined by

$$\mathcal{H}_b = \bigoplus_{2\pi m \leq \phi} e^{2\pi i m y/\ell} f_m(x), \tag{6}$$

where f_m are the eigenfunctions of the chiral Landau Hamiltonian that satisfy spectral boundary condition. $\mathcal{H}_e$, the space of edge states, is the orthogonal complement. The spectrum for the chiral Landau Hamiltonian is shown in Fig. 1.a as a collection of curves plotted as functions of the velocity on the boundary. The bulk spectrum is determined by the left part of the figure i.e. by negative values of the velocity and the edge spectrum by the right part (positive values). The ground state of the bulk spectrum has energy $B/2$ which corresponds to the lowest Landau level in the plane (doubly infinite cylinder). Like it, it is infinitely degenerate. This turns out to be a property of chiral boundary conditions that holds for a large class of billiards: the

ground state of the bulk spectrum has energy $B/2$ and the degeneracy is (an integer close to) the total flux through the billiard. The present case where the total flux is infinite is an example. The bulk ground state is separated by a gap B from the first excited bulk state. For the excited bulk states the situation is more complicated, and one general statement is that the essential bulk spectrum, coincides with the spectrum of the Landau Hamiltonian in the plane: that is, the bulk spectrum differs from the Landau spectrum by at most a discrete set of eigenvalues.

The edge spectrum, in contrast, is, for any finite boundary length ℓ, purely discrete (the essential spectrum is empty). In the thermodynamic limit $\ell \to \infty$ the edge spectrum becomes gapless. The slope of the curves describing the edge spectrum give a linear dispersion with a finite sound velocity as $v_y(\phi, 0) \searrow 0$. In particular, for the lowest edge branch one has, in the limit $\ell \to \infty$, a unique sound velocity for the chiral edge currents:

$$\frac{\partial E_0}{\partial v_y}\Big|_0 = \sqrt{\frac{B}{\pi}} \tag{7}$$

This fixes the k in Eq. (1) in this case. It is worth emphasizing the existence of the discontinuity in derivative between bulk states and the corresponding edge branch as shown in Fig.1.a.

It is instructive to compare the spectral properties of the Chiral Landau Hamiltonian with the Dirichlet Landau model, where one replaces Eq. (5) by the requirement $f_m(0) = 0$ for all m. This too can be solved explicitly in terms of special functions [7] and the spectrum is shown in Fig. 1.b. The corresponding curves are analytic functions. This has some immediate implications: First, there is no sharp line of divide between edge and bulk for the single particle Hamiltonians, second, there is no natural sound velocity because the dispersion law is not linear at small energies, and finally, there is no macroscopic degeneracy of the ground state (or any other state).

The chiral boundary condition Eq. (5) is a close relative of boundary conditions introduced in [4]. APS boundary condition replaces Eq. (5) by

$$\begin{aligned} \left(\frac{d}{dx} - \frac{2\pi m - \phi}{\ell}\right) f_m\Big|_{x=0} &= 0 \quad \text{if } v_y(\phi, 0) \leq 0; \\ f_m\Big|_{x=0} &= 0 \quad \text{if } v_y(\phi, 0) > 0. \end{aligned} \tag{8}$$

That is, the Neumann piece for the edge states is replaced by Dirichlet. Here too there is a sharp divide of the states according to their chirality. But, in APS the putative edge states with the good chirality are forced to have vanishing density near the boundary and tend to be pushed away from the edge. These can not be bona fide edge states. The APS Landau Hamiltonian can be solved explicitly for the problem at hand, and the spectrum is shown in Fig. 1.c. The glaring difference with Fig.1.a is that now the energy curves are *discontinuous*. This discontinuity has undesirable features for studying spectral flows and transport in quantum mechanics.

Consider now the spectral flow resulting from the increase of the threading flux ϕ by a unit of quantum flux: $\phi \to \phi + 2\pi$. By inspection of Fig.1 one sees that all

states in the diagrams move one notch to the left. In the chiral and APS cases which have a clear divide between chiralities we see that each branch of the good chirality looses a state and each branch of the bad chirality gains one. In the chiral case (Fig.1.a) one can follow continuously each state as its chirality changes. In Fig.1.c this is not the case. Chiral boundary conditions therefore give a way of counting the charge being transport from bulk to edge. The same spectral flow takes place for the Dirichlet spectrum except that here what is edge and what is bulk is a vague notion which does not allow for counting the states that move from edge to bulk. In the case of APS the notion of edge and bulk is sharp, but because of the discontinuity of the curves in Fig.1.c there is no way to identify the flow of bulk to edge.

It is also instructive to examine how chiral boundary conditions are related to Laughlin states. As we shall see, Laughlin states for filling fraction $1/M$, M an odd integer, are bulk states with maximal density.

To simplify the notation let us take a cylinder of area 2π, $M = \{(x,y) |\ -1 \leq x \leq 0,\ 0 \leq y < 2\pi\ \}$. We shall take $\phi = 0$ in what follows. The Laughlin state of the (doubly infinite) cylinder for filling fraction $1/M$, with M odd is [9]

$$\psi_L = \prod_{1 \leq j < k \leq N} \left(e^{-z_j} - e^{-z_k}\right)^M \prod_{1 \leq k \leq N} e^{-Bx_k^2/2 + mz_k}. \tag{9}$$

Here $z = x + iy$ and $m \in \mathbb{Z}$. Fix a particle, say $z = z_1$. As a function of z, ψ_L has the form

$$\left(A_1 e^{-M(N-1)z} + A_2 e^{-M(N-2)z} + \ldots\right) e^{-Bx^2/2 + mz} \tag{10}$$

where A_j are independent of z. The chiral boundary conditions for z need to be imposed on the two bounding circles at $x = 0$ and $x = -1$ with opposite orientations. Since ψ_L is in the kernel of D, $(D\psi_L = 0)$, the spectral boundary conditions are automatically satisfied. So, all that needs to be checked is that the velocity on the two bounding circles is anti-chiral. That is:

$$m + B \geq M(N - j) \geq m, \tag{11}$$

for all $1 \leq j \leq N$. $j = N$ sets $m = 0$, and $j = 1$ sets an upper bound on the number of electron that the Laughlin state may accommodate and still satisfy the chiral boundary conditions : $N \leq 1 + B/M$. Recall that the area of the cylinder is 2π, so that B is the total flux in units of quantum flux. In the (thermodynamic) limit of large flux the maximal filling is $N/B \to 1/M$, which is what Laughlin plasma argument gives [8].

The case of other separable billiards, such as a circular disc can be treated in a similar way. For separable billiard of finite area the degeneracy of the chiral bulk ground state can be shown to be related to the total flux. These issues will be described elsewhere [10].

We now turn to the description of the chiral boundary conditions for more general Schrödinger operators and give further motivation for them. It turns out that once chiral boundary conditions have been formulated for the non separable case further generalization to Schrödinger operators with background potential and to multielectron systems where electrons are allowed to interact, follow. For the sake

of simplicity and concreteness we shall stick to one electron billiards. Moreover, to avoid writing complicated formulas, we shall assume that the two dimensional manifold M is (metrically) cylindrical near its boundary ∂M.

It is instructive to formulate the chiral boundary conditions in terms of quadratic forms, and to compare them with the classical boundary conditions, Dirichlet and Neumann. A positive quadratic form, $Q(\varphi)$, on a dense domain, uniquely defines a self-adjoint operator [11]. The nice thing about quadratic forms is that the boundary conditions are part of the form and suggest a physical interpretation. Let $\langle\cdot|\cdot\rangle_M$ stands for the scalar product in $L^2(M)$ and $\langle\cdot|\cdot\rangle_{\partial M}$ for the scalar product on the boundary of M. $C^\infty(M)$ is the space of smooth functions on M. The quadratic form

$$Q(\varphi) = \langle\nabla\varphi|\nabla\varphi\rangle_M + \lambda\,\langle\varphi|\varphi\rangle_{\partial M} \tag{12}$$

with $\varphi \in C^\infty(M)$ and $0 \leq \lambda < \infty$, describes for $\lambda = 0$ the Neumann problem and for $\lambda \to \infty$ the Dirichlet problem for the Laplacian Δ. For finite λ one has elastic boundary conditions. The Neumann problem says that the boundary term gives no penalty (in energy) if there is density on the boundary, while, Dirichlet says that the penalty is large and so finite energies have zero density on the boundary. It is a consequence of the quadratic form and the variational principle that the Dirichlet spectrum have energies above the Neumann spectrum.

Dirichlet and Neumann associate a penalty for density at the boundary. Chiral boundary conditions associate a penalty for a chirality. Since we want edge states (which have positive chirality) to pay a price and bulk states (which have negative chirality) not to affected by the boundary, a quadratic form which does that in the presence of gauge fields is:

$$\begin{aligned} Q_c(\varphi) &= \langle D\varphi|D\varphi\rangle_M + \lambda\left\langle\varphi\middle|v_+\varphi\right\rangle_{\partial M} \\ v_+ &= \begin{cases} v_y & if\ v_y > 0; \\ 0 & otherwise, \end{cases} \end{aligned} \tag{13}$$

where $\varphi \in C^\infty(M)$, $0 \leq \lambda < \infty$ and v_y is the operator of (tangential) velocity on the boundary. Now, in contrast to the Dirichlet-Neumann case discussed above, λ is dimensionless. To see what Eq. (13) implies for the boundary conditions we need to go to the operator and its domain. The domain of $D^\dagger D$ consists of all smooth functions, such that

$$\langle D\varphi|D\cdot\rangle_M + \lambda\left\langle\varphi\middle|v_+\,\cdot\right\rangle_{\partial M}, \tag{14}$$

is a L^2–bounded linear functional. Integration by parts in the variable x leads to

$$\langle D^\dagger D\varphi|\,\cdot\rangle_M + \left\langle(D + \lambda v_+)\varphi\middle|\,\cdot\right\rangle_{\partial M}. \tag{15}$$

For this to define a linear functional, the term on the boundary must vanish identically for all φ in the domain of $D^\dagger D$. If we write $\varphi = \varphi_+ + \varphi_-$, where φ_+ restricted to ∂M belongs to the positive spectral subspace of v_y this domain is defined by: $(d_x + (\lambda - 1)v_y)\varphi_+ = 0$ and $D\varphi_- = 0$. $\lambda = 0$ gives spectral boundary condition for both chiralities. $\lambda = 1$ gives spectral boundary conditions for negative chiralities and Neumann for positive chiralities. This gives the chiral boundary conditions

Eq. (13). $\lambda = \infty$ gives the APS boundary conditions. In principle, one could take λ as a parameter in the theory, fixed by the sound velocity for the edge states. $\lambda = 1$ is distinguished in tending to maximize the density of the edge states at the boundary.

The quadratic form is gauge invariant, non-negative and defines a non-negative, gauge invariant Hamiltonian associated to kinetic energy: $H_L = D^\dagger D \geq 0$.

Chiral Schrödinger Hamiltonians define a self-adjoint eigenvalue problem. This is true irrespective of whether the problem is separable or not; if there is a background scalar potential or not, and even if one considers a one electron theory or a multielectron Hamiltonian. However, only in the separable one particle case, (and slightly more general but still special cases), does one have a clean splitting of the eigenspaces of the Hamiltonian into two pieces: $\mathcal{H}_e$ and $\mathcal{H}_b$. In general, an eigenstate φ will have both a non-zero φ_+ and φ_- piece, and the spectral subspaces do not split cleanly. The best one might expect in the non separable case is that in certain limits eigenstates will have a dichotomy. Namely, either φ_- or φ_+ will be small in the limit for every eigenstate. Examination of simple examples suggests that in the limit of large magnetic fields, $B \to \infty$, there is such an asymptotic splitting. It would be interesting to formulate a splitting principle in the multiparticle Fock space.

In summary: the basic result is that a certain choice of mixed boundary conditions (chiral) gives a clean separation between states identifiable as bulk and edge states.

Acknowledgment

This work is supported in part by the grants from the Israel Academy of Sciences, the DFG, and by the fund for promotion of Research at the Technion. RS acknowledges the hospitality of ITP at the Technion. J. A. thanks L. Sadun for useful discussions.

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