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Heat kernel of integrable billiards in a magnetic field

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Abstract. We present analytical methods to calculate the magnetic response of non-interacting electrons constrained to a domain with boundaries and submitted to a uniform magnetic field. Two different methods of calculation are considered—one involving the large energy asymptotic expansion of the resolvent (Stewartson–Waechter) applies to separable systems, the other based on the small time asymptotic behaviour of the heat kernel (Balian–Bloch). Both methods are in agreement with each other but differ from results previously obtained by Robnik. Finally, the Balian–Bloch multiple scattering expansion is studied and the extension of our results to other geometries is discussed.

1. Introduction

The aim of this work is to present analytical methods for the calculation of the magnetic response of non-interacting electrons constrained to a domain with boundaries and submitted to a uniform magnetic field.

Historically, this problem traces back to the Bohr–van Leeuwen theorem stating the absence of classical orbital magnetism due to the exact cancellation between the bulk and edge magnetizations [1]. Later on, Landau using a quantum approach did show the existence of a finite magnetization [2]. An extension to finite systems was provided by Teller [3] who showed that the Landau magnetization results from an almost cancellation between the bulk and edge contributions. In this work, we shall concentrate on the problem of non-interacting electrons using the semi-infinite plane as a paradigm (our methods can be readily extended to other integrable systems, for instance a disc).

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 integer quantum Hall effect), the high-temperature or weak magnetic field response, such as for instance the orbital diamagnetism, may be obtained using smoothed spectral quantities. 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 Weyl expansion) [4] and to smoothed thermodynamical quantities like the magnetization [5]. This asymptotic expansion of the heat kernel for the semi-infinite plane gives the perimeter correction to the Landau diamagnetism as noted by Robnik [6]. The heat kernel in a uniform magnetic field and a smooth potential was calculated by Prado *et al* [7]. 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

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with those obtained by using the Balian–Bloch [8] expansion. We show (in agreement with more recent works [9]) that the Balian–Bloch method is not very convenient in the presence of a magnetic field due to the fact that several terms in the multiple scattering expansion have to be included in order to obtain just one term in the asymptotic series of the heat kernel. Another asymptotic method we use, following Stewartson and Waechter [10], is powerful enough to give, in principle, all the terms in the asymptotic series for the semi-infinite plane in a magnetic field. However, this latter scheme is applicable only for separable systems while the Balian–Bloch expansion is general. Inspite of the restricted generality of the Stewartson and Waechter's method, we argue that the results have wider validity, in particular that all the coefficients in the asymptotic series are universal in a sense that we shall clarify.

2. Generalities on the resolvent and the heat kernel

The resolvent $G(E)$ of a bounded system is by definition the Laplace transform of the heat kernel $P(t) = \mathrm{Tr}\,\mathrm{e}^{-(1/\hbar)\hat{H}t} = \sum_n \mathrm{e}^{-(1/\hbar)E_n t}$, i.e. formally

$$G(E) = \mathrm{Tr}\,\frac{1}{E+\hat{H}} = \sum_n \frac{1}{E+E_n} \tag{1}$$

where the sum runs over all eigenstates n of the Hamiltonian $\hat{H}$ of the system. This function was extensively studied for the problem of the Laplacian on manifolds with boundaries [11, 12]. As is well known, the small t behaviour of the heat kernel of a particle of mass m moving in a two-dimensional billiard is given by Weyl's formula, $P(t) = (mS/2\pi\hbar t) + \mathrm{O}(t^{-\frac{1}{2}})$, where S is the area of the system; therefore, its Laplace transform is not well defined. A possible way to regularize the Laplace transform is to subtract this leading small t behaviour to $P(t)$ and then take the Laplace transform:

$$g(E) = \frac{1}{\hbar}\int_0^\infty \mathrm{d}t\,\left(P(t) - \frac{mS}{2\pi\hbar t}\right)\mathrm{e}^{-(1/\hbar)Et} \qquad \mathrm{Re}\,(E) > 0. \tag{2}$$

An expression for $g(E)$ valid also for $\mathrm{Re}\,(E) \leqslant 0$ was given by Berry and Howls [4]:

$$g(s=\sqrt{E}) = \lim_{N\to\infty}\left[\sum_{n\leqslant N}\frac{1}{s^2+E_n} - \frac{mS}{2\pi\hbar^2}\ln\left\{\frac{E_N}{s^2}\right\}\right]. \tag{3}$$

It is easy to show that $g(s)$ is related to the density and to the integrated density of states by

$$d(E) = \sum_n \delta(E-E_n) = \frac{mS}{2\pi\hbar^2} - \frac{1}{\pi}\lim_{\varepsilon\to 0^+}\mathrm{Im}\,g(\mathrm{i}\sqrt{E-\mathrm{i}\varepsilon}) \tag{4}$$

$$N(E) = \int_0^E d(\epsilon)\,\mathrm{d}\epsilon = \frac{mSE}{2\pi\hbar^2} - \oint_{C(E)}\frac{\mathrm{d}\epsilon}{2\mathrm{i}\pi}g(s=\mathrm{i}\sqrt{\epsilon}) \tag{5}$$

where the contour $C(E)$ in the complex plane encloses the segment $[0, E]$ of the real axis (such that it contains a finite number of poles of $g(\mathrm{i}\sqrt{\epsilon})$). Both (4) and the fact that $P(t)$ is the Laplace transform of $d(E)$, imply that the two definitions (2) and (3) coincide for $\mathrm{Re}\,(E) > 0$.

Asymptotic expansions of $P(t)$ for small t and of $g(s)$ and $d(E)$ for large s and E, respectively, are related. For example, assuming that we know the Weyl expansion of the resolvent

$$g(s) \sim \sum_{r=1}^{\infty}\frac{c_r}{s^r} \qquad s\to\infty, |\,\mathrm{Arg}(s)| \leqslant \frac{\pi}{2} - \Delta, \Delta > 0 \tag{6}$$

we obtain

$$d(E) \sim \frac{mS}{2\pi\hbar^2} + \frac{1}{\pi\sqrt{E}} \sum_{r=0}^{\infty} \frac{(-1)^r}{E^r} c_{2r+1} \qquad E \to \infty \tag{7}$$

$$P(t) \sim \frac{mS}{2\pi\hbar t} + \sum_{r=1}^{\infty} \frac{c_r}{\Gamma(r/2)} \left(\frac{t}{\hbar}\right)^{(r/2)-1} \qquad t \to 0. \tag{8}$$

The equivalence between (6)–(8) is a consequence of equation (4), the generalized Watson's lemma, and of its reciprocal [13].

As a simple example, the heat kernel and the resolvent associated to the Landau spectrum of a particle moving on a two-dimensional plane in a perpendicular magnetic field B are easily found to be

$$P_\infty(t) = \frac{N_\Phi}{2\sinh(\omega t/2)} \tag{9}$$

and

$$g_\infty(s) = \frac{N_\Phi}{\hbar\omega} \left(\ln\left(-\nu - \frac{1}{2}\right) - \psi(-\nu) \right) \tag{10}$$

where the degeneracy of the levels is $N_\Phi = SB/\Phi_0$ ($\Phi_0 = hc/e$ is the flux quantum), $\omega = eB/mc$ is the cyclotron frequency, $\nu = -(s^2/\hbar\omega) - \frac{1}{2}$ and $\psi(z) = \Gamma'(z)/\Gamma(z)$ is the digamma function. Their asymptotic expansions are

$$\begin{aligned} P_\infty(t) &\sim \frac{N_\Phi}{\omega t} \left(1 - \frac{(\omega t)^2}{24} + \frac{7(\omega t)^4}{5760} + \cdots \right) \\ g_\infty(s) &\sim \frac{N_\Phi}{\hbar\omega} \left(-\frac{1}{24} \left(\frac{\hbar\omega}{s^2}\right)^2 + \frac{7}{960} \left(\frac{\hbar\omega}{s^2}\right)^4 + \cdots \right) \\ d_\infty(E) &\sim \frac{N_\Phi}{\hbar\omega} \qquad \text{(no more terms).} \end{aligned} \tag{11}$$

The last result is obvious because by smoothing out the regular step-like integrated density of states over the energies we obtain a linear function with no higher power-law corrections. Since for any two-dimensional system of surface area S in a uniform magnetic field, $P(t)$ has the same leading (small t) behaviour as $P_\infty(t)$, we may regularize the resolvent by subtracting $P_\infty(t)$ from $P(t)$ and then take the Laplace transform. Such a regularization gives $g(s) - g_\infty(s)$, and can be calculated in the following way.

We define the Wick-rotated retarded Green functions $G^+(t; \boldsymbol{r}, \boldsymbol{r}')$ and $G^+_\infty(t; \boldsymbol{r}, \boldsymbol{r}')$ by $G^+(t; \boldsymbol{r}, \boldsymbol{r}') = G^+_\infty(t; \boldsymbol{r}, \boldsymbol{r}') = 0$ if $t < 0$, and

$$\left(\hat{H} + \hbar\frac{\partial}{\partial t} \right) G^+(t; \boldsymbol{r}, \boldsymbol{r}') = \hbar\delta(t)\delta(\boldsymbol{r} - \boldsymbol{r}') \tag{12}$$

with the additional Dirichlet condition for $G^+(t; \boldsymbol{r}, \boldsymbol{r}')$ on the boundary ∂S of the system:

$$G^+(t; \boldsymbol{r}, \boldsymbol{r}') = 0 \qquad \text{for } \boldsymbol{r} \in \partial S. \tag{13}$$

The Laplace transforms $G(E; \boldsymbol{r}, \boldsymbol{r}')$ and $G_\infty(E; \boldsymbol{r}, \boldsymbol{r}')$, are defined using the same boundary condition (13) and the equation

$$(\hat{H} + E)G(E; \boldsymbol{r}, \boldsymbol{r}') = \delta(\boldsymbol{r} - \boldsymbol{r}'). \tag{14}$$

Then, using (2) and the definition of the heat kernel, we have

$$g(s) - g_\infty(s) = \int_S \mathrm{d}^2\boldsymbol{r}\, (G(s^2; \boldsymbol{r}, \boldsymbol{r}) - G_\infty(s^2; \boldsymbol{r}, \boldsymbol{r})). \tag{15}$$

3. The resolvent for the semi-infinite plane

We aim now to apply (15) in order to extend the method developed by Stewartson and Waechter [10] to the magnetic case. We consider the following set-up. A spinless particle of charge $-e$ ($e > 0$) and mass m moves in the semi-infinite plane. A uniform magnetic field B is applied perpendicular to its surface. Cartesian coordinates are defined such that the x-axis is perpendicular to the boundary and the motion is confined to positive values of x, whereas the y-axis is along the boundary. The Dirichlet boundary condition is imposed at $x = 0$. In order to work with a finite system, we introduce another Dirichlet boundary condition at $x = L_\perp$, where $L_\perp$ is taken so large with respect to the magnetic length $l_B = \sqrt{\hbar c/eB}$ that the corresponding eigenstates do not feel the presence of both boundaries. In this case it is clear that the contributions of the two boundaries to $g(s)$ will be identical (we will check this explicitly later). For the same reason, i.e. working with a finite system, we impose a periodic boundary condition in the y direction, taking L to be the length of the boundary.

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

$$\hat{H} = \frac{1}{2m}\left(\hat{p}_x^2 + \left(\hat{p}_y + \frac{e}{c}Bx\right)^2\right). \tag{16}$$

The Green functions $G(E; \boldsymbol{r}, \boldsymbol{r}')$ and $G_\infty(E; \boldsymbol{r}, \boldsymbol{r}')$ are periodic in $y - y'$ and we can expand them in Fourier series, for example

$$G(E; \boldsymbol{r}, \boldsymbol{r}') = \sum_{p_y} \mathrm{e}^{\mathrm{i}p_y(y-y')/\hbar} G_{p_y}(E; x, x'). \tag{17}$$

The sum runs over $p_y = n_y h/L$, where $n_y \in \mathbb{Z}$. Introducing the dimensionless variables $\tilde{x} = \sqrt{2}x/l_B$, $\tilde{x}_0 = \sqrt{2}p_y/m\omega l_B$, $N'_\Phi = m\omega L^2/2\pi\hbar$ and $\nu = -(E/\hbar\omega) - \frac{1}{2}$, (14) transforms into

$$\left(\frac{\mathrm{d}^2}{\mathrm{d}\tilde{x}^2} - \frac{E}{\hbar\omega} - \frac{1}{4}(\tilde{x} + \tilde{x}_0)^2\right) G_{p_y}(E; \tilde{x}, \tilde{x}') = -\frac{2m}{\hbar^2}(4\pi N'_\Phi)^{-1/2}\delta(\tilde{x} - \tilde{x}'). \tag{18}$$

The solution of this equation together with $G_{p_y}(E; 0, x') = G_{p_y}(E; L_\perp, x') = 0$ can be written as a sum of three terms:

$$G_{p_y}(E; x, x') = -\frac{2m}{\hbar^2\sqrt{4\pi N'_\Phi}}(\tilde{G}_\infty(\nu, \tilde{x}_0; \tilde{x}, \tilde{x}') + \tilde{G}_{1b}(\nu, \tilde{x}_0; \tilde{x}, \tilde{x}') + \tilde{G}_{2b}(\nu, \tilde{x}_0; \tilde{x}, \tilde{x}')). \tag{19}$$

The Green function for unbounded motion $\tilde{G}_\infty(\nu, \tilde{x}_0; \tilde{x}, \tilde{x}')$ is given by

$$\tilde{G}_\infty(\nu, \tilde{x}_0; \tilde{x}, \tilde{x}') = -\frac{\Gamma(-\nu)}{\sqrt{2\pi}} D_\nu(\tilde{x}_> - \tilde{x}_0) D_\nu(\tilde{x}_0 - \tilde{x}_<) \tag{20}$$

where $\tilde{x}_> = \max\{\tilde{x}, \tilde{x}'\}$, $\tilde{x}_< = \min\{\tilde{x}, \tilde{x}'\}$, $D_\nu(u)$ is the parabolic cylinder function (we used the Wronskian [14] $W(D_\nu(u), D_\nu(-u)) = \sqrt{2\pi}/\Gamma(-\nu)$). The last two terms in (19) are respectively the contributions of the boundaries $x = 0$ and $x = L_\perp$ to the Green function. They are obtained by demanding that $G_{p_y}(E; x, x')$ vanishes on the boundaries. However, each boundary is considered separately, i.e. making the Green function vanish on the boundary $x = 0$ we do not impose any condition on the other boundary. Moreover, $G_{p_y}(E; x, x')$ is exponentially small there due to the asymptotic behaviour of the function D_ν for large and positive argument (recall that $\tilde{L}_\perp = \sqrt{2}L_\perp/l_B \gg 1$):

$$\tilde{G}_{1b}(\nu, \tilde{x}_0; \tilde{x}, \tilde{x}) \sim \frac{\Gamma(-\nu)}{\sqrt{2\pi}} \frac{D_\nu(\tilde{x}_0)}{D_\nu(-\tilde{x}_0)} D_\nu^2(\tilde{x} - \tilde{x}_0)$$

$$\tilde{G}_{2b}(\nu, \tilde{x}_0; \tilde{x}, \tilde{x}) \sim \frac{\Gamma(-\nu)}{\sqrt{2\pi}} \frac{D_\nu(\tilde{L}_\perp - \tilde{x}_0)}{D_\nu(\tilde{x}_0 - \tilde{L}_\perp)} D_\nu^2(\tilde{x}_0 - \tilde{x}). \tag{21}$$

Since we are interested in the limit $L \to \infty$, we can now replace the sum over p_y in (17) by an integral. We deduce that $\tilde{G}_{1b}(\nu, \tilde{x}_0; \tilde{x}, \tilde{x})$ and $\tilde{G}_{2b}(\nu, \tilde{x}_0; \tilde{x}, \tilde{x})$ give the same contribution to (15), which can be expressed using known [14] integrals of the function D_ν as

$$\begin{aligned} g(s) - g_\infty(s) &= \frac{\Gamma(-\nu)\sqrt{N'_\Phi}}{\hbar\omega\sqrt{8\pi^2}} \int_{-\infty}^{\infty} \mathrm{d}\tilde{x}_0 \, \frac{D_\nu(\tilde{x}_0)}{D_\nu(-\tilde{x}_0)} \\ &\quad \times \left(D_\nu(-\tilde{x}_0) \frac{\partial D'_\nu}{\partial \nu}(-\tilde{x}_0) - D'_\nu(-\tilde{x}_0) \frac{\partial D_\nu}{\partial \nu}(-\tilde{x}_0) \right) \\ &= \frac{\sqrt{N'_\Phi}}{\sqrt{4\pi}\hbar\omega} \lim_{\tilde{X}_0 \to \infty} \left(\frac{\partial}{\partial \nu} \int_{-\tilde{X}_0}^{\tilde{X}_0} \mathrm{d}\tilde{x}_0 \, \ln D_\nu(-\tilde{x}_0) - \tilde{X}_0 \psi(-\nu) \right). \end{aligned} \tag{22}$$

This is the resolvent for the semi-infinite plane. In the infinitely large strip geometry, the corresponding $g(s) - g_\infty(s)$ is twice this result.

Formula (22) might be understood more intuitively as follows. The integrated density of states $N(E)$ counts the number of zeros of the wavefunction at the origin $D_{(\epsilon/\hbar\omega)-\frac{1}{2}}(\tilde{x}_0)$, for all $\tilde{x}_0$ and all energies ϵ up to $\epsilon = E$:

$$N(E) = \sum_{p_y} \oint_{C(E)} \frac{\mathrm{d}\epsilon}{2\pi\mathrm{i}} \frac{\partial}{\partial \epsilon} \ln D_{(\epsilon/\hbar\omega)-\frac{1}{2}}(\tilde{x}_0). \tag{23}$$

The sum and the integral cannot be inverted since there are infinitely many states. However, we can formally subtract from $N(E)$ the integrated density of states of the infinite plane which we write

$$N_\infty(E) = \frac{1}{2} \sum_{p_y} \sum_{n_x} \theta\left(E - \hbar\omega\left(n_x + \frac{1}{2}\right)\right) = -\frac{1}{2\hbar\omega} \sum_{p_y} \oint_{C(E)} \frac{\mathrm{d}\epsilon}{2\pi\mathrm{i}} \psi\left(-\frac{\epsilon}{\hbar\omega} + \frac{1}{2}\right) \tag{24}$$

(a factor $\frac{1}{2}$ is introduced since we neglected the second boundary contribution in (23)). Using (5) we obtain

$$g(s) - g_\infty(s) = \frac{1}{\hbar\omega} \sum_{p_y} \left(\frac{\partial}{\partial \nu} \ln D_\nu(\tilde{x}_0) - \frac{1}{2}\psi(-\nu) \right). \tag{25}$$

Replacing here the sum over p_y by an integral we obtain (22). The heat kernel is found by performing an inverse Laplace transform on (22) or (25).

It is worth noticing that $g(\sqrt{E})$ and $P(t)$ have the following forms:

$$\begin{aligned} \hbar\omega g(\sqrt{E}) &= N_\Phi \tilde{g}_\infty\left(\frac{E}{\hbar\omega}\right) + \sqrt{N'_\Phi}\tilde{g}_S\left(\frac{E}{\hbar\omega}\right) \\ P(t) &= N_\Phi \tilde{P}_\infty(\omega t) + \sqrt{N'_\Phi}\tilde{P}_S(\omega t) \end{aligned} \tag{26}$$

where $N_\Phi = m\omega L L_\perp/2\pi\hbar$, $N'_\Phi = m\omega L^2/2\pi\hbar$ and none of the functions denoted by tilde depend explicitly on B, L or $L_\perp$. The boundary term is proportional to $\sqrt{N'_\Phi}$ and is smaller than the bulk term by a factor of order $1/\sqrt{N_\Phi}$ for $L_\perp \sim L$. For finite lengths L of the boundary, there are exponentially small correction terms in (22) and (26) due to the error introduced by replacing the sum in (17) by an integral. Neglecting these small corrections, the asymptotic expansion of the heat kernel and of the density of states in terms of $h_{\mathrm{eff}} = 1/N'_\Phi$, as a small parameter (assuming large fields or large systems), has two terms only. This is due to the straight boundary and there will be more terms if the boundary has a non-zero curvature.

We also check our result in the opposite limit $B \to 0$. Since $\tilde{P}_\infty(\tau) \sim \tau^{-1}$ as $\tau \to 0$ (see (10)) and, as we shall see in the next section, $\tilde{P}_s(\tau) \sim -\frac{1}{4}\tau^{-1/2}$, we have

$$P(B=0,t) \simeq \frac{mLL_\perp}{2\pi\hbar t} - \frac{L}{4}\sqrt{\frac{m}{2\pi\hbar t}}.$$

This equation is true up to exponentially small terms for large L and $L_\perp$ (or equivalently for small t); it agrees with the well known observation that, when the curvature of the boundary is zero everywhere, the coefficients c_r in the Weyl expansion (8) vanish for $r \geqslant 2$.

The results of this section may be extended to any separable system provided it reduces to a one-dimensional Sturm–Liouville problem. As an example, we derive in the appendix the resolvents of a particle moving in a disc with and without a magnetic field.

4. Weyl expansions of the resolvent and the heat kernel

In this section we shall derive asymptotic expressions for the heat kernel and the resolvent using equation (25). For large positive energies (large negative ν) and large $\tilde{x}_0$ the Darwin asymptotic expansion (basically WKB expansion of the wavefunction) of the parabolic cylinder function [15, 16] is

$$\ln D_\nu(\tilde{x}_0) \sim \frac{\ln 2\pi}{4} - \frac{1}{2}\ln\Gamma(-\nu) - \theta(\tilde{x}_0, a) - \frac{1}{4}\ln(\tilde{x}_0^2 + 4a) + \sum_{s=1}^{\infty} \frac{(-1)^s d_{3s}}{(\sqrt{\tilde{x}_0^2 + 4a})^{3s}} \tag{27}$$

where $\theta(\tilde{x}_0, a)$ is an odd function of $\tilde{x}_0$, $a = E/\hbar\omega > 0$ 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 $\tilde{x}_0$ in (25) over a symmetric interval, only even functions of $\tilde{x}_0$ do contribute. The first three even-indexed coefficients d_{3s} are given respectively by [15]

$$d_6 = \frac{3}{4}\tilde{x}_0^2 - 2a \qquad d_{12} = \frac{153}{8}\tilde{x}_0^4 - 186a\tilde{x}_0^2 + 80a^2$$

and

$$d_{18} = \frac{6381}{4}\tilde{x}_0^6 - 29862a\tilde{x}_0^4 + 62292a^2\tilde{x}_0^2 - \frac{31232}{3}a^3.$$

Using (25) and (11) we obtain the asymptotic expansion of the resolvent

$$g(s=\sqrt{\hbar\omega a}) \sim \frac{N_\Phi}{\hbar\omega}\left(-\frac{1}{24a^2} + \frac{7}{960a^4} + \cdots\right) - \frac{\sqrt{\pi N'_\Phi}}{4\hbar\omega}\left(\frac{1}{\sqrt{a}} - \frac{9}{256a^{5/2}} + \frac{2625}{262144a^{9/2}} - \frac{241197}{2^{25}a^{13/2}} + \cdots\right). \tag{28}$$

Similarly, the Weyl expansion of the heat kernel is derived using (8)

$$P\left(t=\frac{\tau}{\omega}\right) = \frac{N_\Phi}{\tau}\left(1 - \frac{\tau^2}{24} + \frac{7\tau^4}{5760} - \cdots\right) - \frac{\sqrt{N'_\Phi}}{4\sqrt{\tau}}\left(1 - \frac{3\tau^2}{64} + \frac{25\tau^4}{16384} - \frac{7309\tau^6}{315\times 2^{20}} + \cdots\right). \tag{29}$$

These expansions could, in principle, be continued indefinitely, by calculating recursively the coefficients d_{6s}.

It is instructive to compare the expression (29) with its counterpart at $B = 0$. The heat kernel in the absence of magnetic field is simply obtained from (29) by taking the argument of the analytic function of τ in each set of parentheses to be zero. Two terms are obtained, the area and the perimeter. Since these terms are known to be general for the case of billiards irrespective of their integrability, we suggest that our result will apply to any billiard in a uniform magnetic field (although it was derived for an integrable system). It is worth emphasizing that the two terms in (29) are only part of the asymptotic expansion for a general magnetic billiard. There should be additional terms proportional to the integrals over the curvature and its derivatives [4, 10]. We conjecture that the generalization of the heat kernel expansion obtained for a two-dimensional billiard without magnetic field to the case of magnetic billiard consists of multiplying each term of that expansion by an analytic function of τ. These functions should be universal for all flat two-dimensional billiards with smooth boundaries. Similar conclusions have been obtained for the related case of a Aharonov–Bohm billiard [17].

Note that in the case of a particle in the infinite plane in a perpendicular field confined by a harmonic potential, Prado *et al* [7] found the coefficient c_2 in (8) to be $\alpha + \beta B^2$, where α and β are constants depending on the potential which corresponds to the geometric features of the boundary in our problem.

5. The Balian–Bloch method

The small time asymptotic expansion of the heat kernel can also be obtained using a method suggested by Balian and Bloch [8]. It consists of 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 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 [8].

The Green function for the Dirichlet problem in a domain S with a boundary ∂S in absence of magnetic field is written as a sum of two terms:

$$G(E;\boldsymbol{r},\boldsymbol{r}') = G_\infty(E;\boldsymbol{r},\boldsymbol{r}') + G_S(E;\boldsymbol{r},\boldsymbol{r}') \tag{30}$$

where each term on the right-hand side satisfies (14) in which $\hat{H} = -(\hbar^2/2m)\Delta$ is a Laplacian. The first term is the infinite plane Green function while the second is specified by the boundary condition $G_S(E;\boldsymbol{r},\boldsymbol{r}') = -G_\infty(E;\boldsymbol{r},\boldsymbol{r}')$ for $\boldsymbol{r}$ on ∂S. This boundary term is expressed in terms of an unknown density $\mu_E(\boldsymbol{\alpha},\boldsymbol{r})$ as

$$G_S(E;\boldsymbol{r},\boldsymbol{r}') = \int_{\partial S} \mathrm{d}\sigma_\alpha \, \frac{\partial G_\infty(E;\boldsymbol{r},\boldsymbol{\alpha})}{\partial n_\alpha} \mu_E(\boldsymbol{\alpha},\boldsymbol{r}') \tag{31}$$

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

$$\frac{m}{\hbar^2}\mu_E(\boldsymbol{\alpha},\boldsymbol{r}') = -G_\infty(E;\boldsymbol{\alpha},\boldsymbol{r}') - \int_{\partial S} \mathrm{d}\sigma_\beta \, \frac{\partial G_\infty(E;\boldsymbol{\alpha},\boldsymbol{\beta})}{\partial n_\beta} \mu_E(\boldsymbol{\beta},\boldsymbol{r}') \tag{32}$$

where $\boldsymbol{\alpha},\boldsymbol{\beta},\ldots$ are arbitrary points on the boundary ∂S, $\mathrm{d}\sigma_\beta$ is the boundary differential element, and $\partial/\partial n_\beta$ is the normal derivative at the point $\boldsymbol{\beta}$ with the normal oriented towards the interior of the domain. Solving iteratively the integral equation (32) for the density $\mu_E(\boldsymbol{\alpha},\boldsymbol{r}$, the following multiple reflection expansion is obtained for the Green function:

$$\begin{aligned} G(E;\boldsymbol{r},\boldsymbol{r}') = {} & G_\infty(E;\boldsymbol{r},\boldsymbol{r}') - \frac{\hbar^2}{m}\int_{\partial S} \mathrm{d}\sigma_\alpha \, \frac{\partial G_\infty(E;\boldsymbol{r},\boldsymbol{\alpha})}{\partial n_\alpha} G_\infty(E;\boldsymbol{\alpha},\boldsymbol{r}') \\ & + \left(\frac{\hbar^2}{m}\right)^2 \int_{\partial S} \mathrm{d}\sigma_\alpha \, \mathrm{d}\sigma_\beta \frac{\partial G_\infty(E;\boldsymbol{r},\boldsymbol{\alpha})}{\partial n_\alpha} \frac{\partial G_\infty(E;\boldsymbol{\alpha},\boldsymbol{\beta})}{\partial n_\beta} G_\infty(E;\boldsymbol{\beta},\boldsymbol{r}') - \cdots . \end{aligned} \tag{33}$$

Using the time-dependent Green function $G^+(t;\boldsymbol{r},\boldsymbol{r}')$ introduced in section 4, we calculate the heat kernel $P(t)=\int_S \mathrm{d}^2\boldsymbol{r}\, G^+(t;\boldsymbol{r},\boldsymbol{r})$. The multiple expansion of $G^+(t;\boldsymbol{r},\boldsymbol{r}')$ is

$$\begin{aligned} G^+(t;\boldsymbol{r},\boldsymbol{r}') &= G^+_\infty(t;\boldsymbol{r},\boldsymbol{r}') - \frac{\hbar}{m}\int_{\partial S}\mathrm{d}\sigma_\alpha \int_0^t \mathrm{d}\tau\, \frac{\partial G^+_\infty(t-\tau;\boldsymbol{r},\boldsymbol{\alpha})}{\partial n_\alpha} G^+_\infty(\tau;\boldsymbol{\alpha},\boldsymbol{r}') \\ &\quad + \left(\frac{\hbar}{m}\right)^2 \int_{\partial S}\mathrm{d}\sigma_\alpha\,\mathrm{d}\sigma_\beta \int_0^t \mathrm{d}\tau_1 \int_0^{\tau_1}\mathrm{d}\tau_2\, \frac{\partial G^+_\infty(t-\tau_1;\boldsymbol{r},\boldsymbol{\alpha})}{\partial n_\alpha} \\ &\quad \times \frac{\partial G^+_\infty(\tau_1-\tau_2;\boldsymbol{\alpha},\boldsymbol{\beta})}{\partial n_\beta} G^+_\infty(\tau_2;\boldsymbol{\beta},\boldsymbol{r}') - \cdots. \end{aligned} \tag{34}$$

This approach was applied in this form to the case of a uniform magnetic field perpendicular to the domain S [6]. However, care must be taken since at each order of the multiple reflection expansion we obtain a term which is not gauge invariant. This problem may be easily corrected by introducing the covariant derivative $\partial/\partial n_\alpha - (\mathrm{i}e/\hbar c)A_n(\boldsymbol{\alpha})$ instead of the usual $\partial/\partial n_\alpha$. 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, it should be taken into account.

Let us, therefore, apply the Balian and Bloch method to the semi-infinite plane in a uniform magnetic field. The Green function for the infinite plane is given by

$$G^+_\infty(t;\boldsymbol{r},\boldsymbol{r}') = \frac{m\omega}{4\pi\hbar\sinh(\omega t/2)}\exp\left[-\frac{m\omega}{4\hbar}(\boldsymbol{r}-\boldsymbol{r}')^2\coth\frac{\omega t}{2} - \frac{\mathrm{i}m\omega}{2\hbar}(y-y')(x+x')\right]. \tag{35}$$

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:

$$P(t) = P_\infty(t) - \frac{L}{8}\sqrt{\frac{2m}{\pi\hbar t}} + \frac{L}{8}\sqrt{\frac{2m}{\pi\hbar t}}\frac{3}{64}\omega^2 t^2 - \cdots \tag{36}$$

in accordance with the result (29) obtained previously. This, however, disagrees with Robnik's calculation [6]. In his work this author assumed that, in the case of a zero-curvature boundary, the one-reflection term contains all the corrections due to the boundary (as for the problem without magnetic field). However, as already noted by John and Suttorp [9], higher-order terms cannot be neglected in calculating physical quantities in the geometry with straight boundaries in the presence of a magnetic field. We also emphasize 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 $(2n+1)$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. Perimeter corrections to the Landau diamagnetism

In this section we apply the previous results in order to compute the magnetic susceptibility of a gas of independent electrons in a strip of very large width $L_\perp$.

Let us first consider the case of a non-degenerate gas at temperature $T = 1/k_B\beta$. The heat kernel $P(t)$ when considered a function of an inverse temperature $t = \tau/\omega = \hbar\beta$ coincides with the one-electron (canonical) partition function (which we denote by $Z(\beta)$ in the following). If N is the electronic density (per unit area) and $\mu_B = e\hbar/2mc$ the Bohr magneton, the magnetic susceptibility of the ideal gas is given by

$$\chi = \lim_{\tau\to 0} 4N\mu_B^2\beta \frac{\partial^2}{\partial\tau^2}\ln Z. \tag{37}$$

Using the expansion (29) of $P(t)$ we obtain the weak field susceptibility,

$$\chi = -\frac{1}{3}N\beta\mu_B^2\left(1 - \frac{\lambda_T}{16L_\perp}\left(1-\frac{\lambda_T}{2L_\perp}\right)^{-1}\right) \tag{38}$$

where $\lambda_T = \sqrt{\pi\beta\hbar^2/2m}$ is the de Broglie thermal length. As in [6] the correction to the Landau diamagnetic susceptibility $\chi_\infty = -\frac{1}{3}N\beta\mu_B^2$ is paramagnetic, but is smaller by one order of magnitude. Our result agrees with numerical calculations performed by van Ruitenbeck and van Leeuwen [18].

For a degenerate electron gas of Fermi energy E_F, the relation between the susceptibility and the canonical partition function is different [5]. In the grand-canonical ensemble, χ is given by

$$\chi = -\lim_{B\to 0}\frac{1}{S}\frac{\partial^2\Omega(E_F)}{\partial B^2} \tag{39}$$

with $\Omega(E_F)$ being the thermodynamic potential. The thermodynamic potential at zero temperature $\Omega_0(E_F)$ is related to the partition function (heat kernel) through [5]

$$\Omega_0(E_F) = -\int_{-i\infty+0+}^{i\infty+0+}\frac{d\beta}{2\pi i}e^{\beta E_F}\beta^{-2}Z(\beta). \tag{40}$$

Using (26) we obtain

$$\Omega_0(E_F) = -\frac{mS}{2\pi}\int_{-i\infty+0+}^{i\infty+0+}\frac{d\tau}{2\pi i}e^{\tau E_F/\hbar\omega}\left(\omega^2\tau^{-2}\tilde{P}_\infty(\tau) + \sqrt{\frac{2\pi\hbar}{mL_\perp^2}}\omega^{3/2}\tau^{-2}\tilde{P}_S(\tau)\right). \tag{41}$$

Replacing in this equation the Weyl expansions (29) of $\tilde{P}_\infty(\tau)$ and $\tilde{P}_S(\tau)$ amounts to neglecting all oscillating contributions due to periodic orbits in $\Omega_0(E_F)$. However, even though those oscillating terms in the thermodynamic potential may give at very low temperature the largest corrections to the Landau diamagnetism, they are exponentially damped by temperature [19, 20] (more precisely, the contribution of each periodic orbit is damped by the factor $(2\pi rmL_\perp/\hbar^2\beta k_F)\sinh^{-1}(2\pi rmL_\perp/\hbar^2\beta k_F)$, where r is the number of repetitions of the orbit and $k_F = \sqrt{2mE_F}/\hbar$ is the Fermi wavevector). For temperatures $\hbar^2k_F/mL_\perp \ll k_BT \ll E_F$, we can neglect these oscillating contributions and we have at small field

$$\chi \simeq \bar{\chi} = -\frac{e^2}{24\pi mc^2}\left(1 - \frac{9}{16}\frac{1}{L_\perp k_F}\right). \tag{42}$$

Here again the correction is paramagnetic and coincides with perturbative calculations [20].

The expressions (38) and (42) give the magnetic susceptibilities of a semi-infinite plane regularized to have a finite width $L_\perp$ for small fields B such that $L_\perp \gg l_B$. The second term in these equations has to be multiplied by two for the case of a finite (but very large) strip instead of the semi-infinite plane.

The susceptibilities (38) and (42) give the perimeter corrections to the Landau diamagnetism for a general billiard of surface S and smooth boundary of length L, with $L_\perp = S/L$ (although the method of Stewartson and Waechter works only for integrable systems, the fact that it coincides with the more general Balian–Bloch expansion suggests that our results are general). However, for a generic billiard this correction is not the only one (although it is the leading one), and presumably other terms due to the curvature of the boundary will appear.

7. Conclusion

We have derived exact relations for the resolvent and the heat kernel using the special case of the semi-infinite plane in a uniform magnetic field. These relations are convenient starting points for an asymptotic expansion, using the WKB approximation for the wavefunctions. The validity of the method presented extends beyond the special case of this special geometry and it works for any separable system. Our main result is the closed expression for the boundary term of the heat kernel whose asymptotic expansion can be calculated recursively as an infinite series. The first terms of this series were also obtained using the Balian–Bloch multiple scattering expansion, which in practice appears to be less convenient than the method of Stewartson and Waechter in the presence of a magnetic field. Then, the perimeter corrections to the Landau diamagnetism are obtained both in the high-temperature limit and for a degenerate gas.

Various properties of the heat kernels of Laplacians on manifolds have been extensively investigated starting (among others) from the work of Kac [11] in order to relate the spectral and geometrical descriptions [12]. Our results could be viewed as an extension of these works towards the case of magnetic billiards. For a straight boundary, the effect of the magnetic field is to add an infinite series to the bare perimeter term and this is, in some sense, equivalent to an effective curvature of the boundary. We conjecture that the perimeter term of a general magnetic billiard will be equal to that of a straight boundary. More generally, the boundary has a curvature and therefore another length scale enters the problem and is coupled to the cyclotron radius. This leads to additional terms in the asymptotic expansion of the heat kernel. Whether those terms appear as a scaling function of both the cyclotron radius and the curvature is an important issue which deserves further study.

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Appendix

Consider a particle confined to a disc of radius R. The energies (imposing Dirichlet boundary conditions) are the solutions of the equation $J_l(kR) = 0$, where l is the angular momentum quantum number and $k^2 = 2mE/\hbar^2$ is the momentum. The number $N(E)$ of zeros is equal to the integral of the logarithmic derivative of the Bessel function:

$$N(E) = \sum_l \oint_{C(E)} \frac{\mathrm{d}\epsilon}{2\pi \mathrm{i}} \frac{(\mathrm{d}J_l(kR)/\mathrm{d}\epsilon)}{J_l(kR)}. \tag{A.1}$$

Then according to the method that we developed for the semi-infinite plane geometry, we obtain for the resolvent

$$G(E) = \sum_l \frac{m}{\hbar^2 k} \frac{(\mathrm{d}I_l(kR)/\mathrm{d}k)}{I_l(kR)} \tag{A.2}$$

which coincides with the result of Stewartson and Waechter [10] when subtracting the resolvent corresponding to the infinite plane.

For the corresponding problem in the presence of a magnetic field, the energies are solutions of ${}_1F_1((l + |l| + 1)/2 - (E/\hbar\omega); 1 + |l|; N_\Phi) = 0$, where $N_\Phi = SB/\Phi_0$ and ${}_1F_1(a; c; u)$ is the confluent hypergeometric function [16]. The counting function is now

$$N(E) = \sum_l \oint_{C(E)} \frac{\mathrm{d}\epsilon}{2\pi \mathrm{i}} \frac{(\mathrm{d}_1F_1((l + |l| + 1)/2 - (\epsilon/\hbar\omega); 1 + |l|; N_\Phi)/\mathrm{d}\epsilon)}{{}_1F_1((l + |l| + 1)/2 - (\epsilon/\hbar\omega); 1 + |l|; N_\Phi)} \tag{A.3}$$

and the resolvent

$$G(E) = \sum_l \frac{(\mathrm{d}_1F_1((l + |l| + 1)/2 + (E/\hbar\omega); 1 + |l|; N_\Phi)/\mathrm{d}E)}{{}_1F_1((l + |l| + 1)/2 + (E/\hbar\omega); 1 + |l|; N_\Phi)}. \tag{A.4}$$

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.

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