A TRACE FORMULA FOR MULTIDIMENSIONAL SCHRÖDINGER OPERATORS

F. Gesztesy[1], H. Holden[2], B. Simon[3], and Z. Zhao[1]

Abstract. We prove multidimensional analogs of the trace formula obtained previously for one-dimensional Schrödinger operators. For example, let V be a continuous function on $[0,1]^\nu \subset \mathbb{R}^\nu$. For $A \subset \{1,\dots,\nu\}$, let $-\Delta_A$ be the Laplace operator on $[0,1]^\nu$ with mixed Dirichlet-Neumann boundary conditions

$$\begin{aligned} \varphi(x) &= 0, \qquad x_j = 0 \text{ or } x_j = 1 \quad \text{for } j \in A, \\ \frac{\partial\varphi}{\partial x_j}(x) &= 0, \qquad x_j = 0 \text{ or } x_j = 1 \quad \text{for } j \notin A. \end{aligned}$$

Let $|A| =$ number of points in A. Then we'll prove that

$$\operatorname{Tr}\Bigg(\sum_{A\subset\{1,\dots,\nu\}} (-1)^{|A|} e^{-t(-\Delta_A+V)}\Bigg) = 1 - t\langle V\rangle + o(t) \quad \text{as } t \downarrow 0$$

with $\langle V\rangle$ the average of V at the 2^ν corners of $[0,1]^\nu$.

§1. Introduction

This paper is devoted to extensions of the trace formula for the ODE $-\frac{d^2}{dx^2}+V(x)$ to the corresponding PDE, $-\Delta + V(x)$. The simplest of all the one-dimensional results is the trace formula [1,6] for the periodic case. Suppose V is a C^1 function on $\mathbb{R}$ obeying $V(x+1) = V(x)$. Let $E_1 < E_4 \leq E_5 < E_8 \leq E_9 < \cdots$ be the eigenvalues of the operator on $L^2([0,1])$

$$-\frac{d^2}{dx^2} + V \tag{1}$$

[1] Department of Mathematics, University of Missouri, Columbia, MO 65211. E-mail for F.G.: mathfg
@mizzou1.missouri.edu E-mail for Z.Z.: mathzz@mizzou1.missouri.edu

[2] Department of Mathematical Sciences, The Norwegian Institute of Technology, University of Trondheim, N-7034 Trondheim, Norway. E-mail: holden@imf.unit.no

[3] Division of Physics, Mathematics, and Astronomy, California Institute of Technology, 253-37, Pasadena, CA 91125. This material is based upon work supported by the National Science Foundation under Grant No. DMS-9101715. The Government has certain rights in this material.

To be submitted to *J. Amer. Math. Soc.*

with periodic boundary conditions (call the operator H^P) and $E_2 \leq E_3 < E_6 \leq E_7 < \cdots$ the eigenvalues of (1) with antiperiodic boundary conditions (call the operator H^A). Let $\mu_1(x) < \mu_2(x) < \cdots$ be the eigenvalues of the operator (1) on $L^2([x, x+1])$ with $u(x) = u(x+1) = 0$ Dirichlet boundary conditions (call the operator H_x^D). Then:

$$V(x) = E_0 + \sum_{n=1}^{\infty} \big[E_{2n} + E_{2n-1} - 2\mu_n(x)\big], \quad x \in [0,1]. \tag{2}$$

One way (see, e.g., [8]) of proving (2) is to derive a heat kernel asymptotic relation

$$\mathrm{Tr}(e^{-tH^P} + e^{-tH^A} - 2e^{-tH_x^D}) = 1 - tV(x) + o(t) \tag{3}$$

from which (2) follows from the known convergence of

$$\sum_{n=1}^{\infty} |E_{2n} - E_{2n-1}| < \infty \tag{4}$$

and the relation

$$E_{2n-1} \leq \mu_n(x) \leq E_{2n}.$$

Equation (3) can be viewed as an Abelian summation method applied to (2) and holds even in cases where (4) diverges (e.g., if $V(x) =$ the characteristic function of $\bigcup_{n=-\infty}^{\infty} [n - \frac{1}{4}, n + \frac{1}{4}]$).

Recently, we have described versions of (3) for arbitrary, not necessarily periodic, V's by using other boundary conditions, see [3,2]. For example, if H is (1) on all of $(-\infty, \infty)$ and H_x^D is (1) on $L^2(-\infty, x) \oplus L^2(x, \infty)$ with $u(x) = 0$ Dirichlet boundary conditions, then we proved that

$$2\mathrm{Tr}\big(e^{-tH} - e^{-tH_x^D}\big) = 1 - tV(x) + o(t), \quad x \in \mathbb{R} \tag{5}$$

so as long as x is a point of Lebesgue continuity of V and V is bounded from below and locally L^1.

One of our main accomplishments here is to extend (5) to higher dimensions. Let H_x^N denote the operator with Neumann boundary conditions and suppose V is even about x, that is, $V(x-y) = V(x+y)$, $y \in \mathbb{R}$. Then

$$e^{-tH_x^Q}(x+y, x+z) = e^{-tH}(x+y, x+z) \pm e^{-tH}(x+y, x-z)$$

if $yz > 0$ and the $-$ is used for $Q = D$ and $+$ for $Q = N$. (Here and in the remainder of this paper $e^{-tH}(x,y)$, $t > 0$ denotes the integral kernel of the semigroup e^{-tH}.) From this it follows that $\mathrm{Tr}(e^{-tH} - e^{-tH_x^D}) = \mathrm{Tr}(e^{-tH_x^N} - e^{-tH})$ and so (5) becomes

$$\mathrm{Tr}\big(e^{-tH_x^N} - e^{-tH_x^D}\big) = 1 - tV(x) + o(t), \quad x \in \mathbb{R}. \tag{6}$$

But it is easy to see that (6) for V even about x implies it for arbitrary V since the operators break up into direct sums (see Lemma 2.1 below).

It is (6) that we will generalize to ν dimensions. Explicitly, given $A \subset \{1, \dots, \nu\}$, let $H_{A;x}$ be defined as follows: Let B_α, $\alpha \subset \{1, \dots, \nu\}$ be the 2^ν blocks obtained by removing the hyperplanes $P_j^{(x)} := \{y \in \mathbb{R}^\nu \mid y_j = x_j\}$ from $\mathbb{R}^\nu$, that is, $B_\alpha = \{x \in \mathbb{R}^\nu \mid x_i > 0 \text{ if } i \in \alpha,\, x_i < 0 \text{ if } i \notin \alpha\}$. $H_{A;x}$ is then defined to be the operator on $\oplus L^2(B_\alpha)$ with Dirichlet boundary conditions on $\{P_j^{(x)}\}_{j \in A}$ and Neumann boundary conditions on $\{P_j^{(x)}\}_{j \notin A}$.

Explicitly, for each $\alpha = 1, \dots, 2^\nu$, let $\mathcal{D}_{\alpha;x}^{(A)}$ be the set of functions, φ, on B_α which are C^∞ on B_α^{int}, with derivatives continuous up to ∂B_α with bounded support and which obey the boundary conditions:

$$\begin{aligned} \varphi(y) &= 0, \qquad y \in P_j^{(x)} \quad \text{for } j \in A, \\ \frac{\partial \varphi}{\partial y_j}(y) &= 0, \qquad y \in P_j^{(x)} \quad \text{for } j \notin A. \end{aligned}$$

Obviously, $\mathcal{D}_{\alpha;x}^{(A)}$ is dense in $L^2(B_\alpha)$. Then $\varphi \mapsto -\triangle \varphi$ is essentially self-adjoint on $\mathcal{D}_{\alpha,x}^{(A)}$, $-\triangle_A$ is the direct sum of these operators on $\oplus L^2(B_\alpha)$, and $H_{A;x} = -\triangle_A \dot{+} V$ as a form sum.

We will prove (see Theorem 4.1) that

$$\operatorname{Tr}\biggl(\sum_{A \subset \{1,\dots,\nu\}} (-1)^{|A|} \exp(-tH_{A;x}) \biggr) = 1 - tV(x) + o(t), \quad x \in \mathbb{R}^\nu. \tag{7}$$

(Note that for $A = \{1, \dots, \nu\}$ resp. $A = \emptyset$, $H_{A;x}$ has exclusively Dirichlet resp. Neumann boundary conditions on the hyperplanes $P_j^{(x)}$, $1 \le j \le \nu$.)

The paper is laid out as follows. In §2, we'll use the method of images to reduce (7) to the study of integrals of the form

$$2^\nu \int_{\mathbb{R}^\nu} \exp(-tH)(y, -y)\, d^\nu y, \tag{8}$$

where $H = -\triangle + V$ is a Schrödinger operator in $L^2(\mathbb{R}^\nu)$ without any boundary conditions. In §3, we introduce a Gaussian process that provides a concise Feynman-Kac type formula for integrals of the form (8), and we'll prove (7) in §4. We'll discuss the periodic version of (7) in §5, then prove an abelianized version of a recent conjecture of Lax [5] that motivated our work. Finally, in §6, we'll make a few remarks on the issue of going beyond Abelian sums in the periodic case.

§2. The Method of Images

We begin with some small arguments to simplify notation and some later details. First, without loss, we'll suppose $x = 0$, that is, all boundary conditions are on planes through 0 and the final formula is for $V(0)$. Let then P_j be the coordinate plane $\{x \in \mathbb{R}^\nu \mid x_j = 0\}$ and let $H_A \equiv H_{A;0}$. Let π_j be the reflection in P_j, that is,

$$\begin{aligned} (\pi_j x)_i &= x_i, \qquad i \neq j \\ &= -x_j, \qquad i = j. \end{aligned}$$

Call V symmetric if and only if $V \circ \pi_j = V$ for all j. For $\alpha \subset \{1, \dots, \nu\}$, let B_α be the blocks introduced previously. Let V_α be that symmetric function with $V_\alpha = V$ on B_α. Because of symmetry of V_α for each A, $\exp(-t(-\Delta_A + V_\alpha))$ is a direct sum of 2^ν pieces (acting on the different $L^2(B_\beta)$) and each of the pieces is unitarily equivalent to a single operator, $P_{A;\alpha,t}$. On the other hand, $\exp(-tH_A)$ is also a direct sum, clearly unitarily equivalent to $\bigoplus_{\alpha\subset\{1,\dots,\nu\}} P_{A;\alpha,t}$. It follows that:

Lemma 2.1. *To prove* (7), *it suffices to suppose $x = 0$ and that V is symmetric.*

So, henceforth, we can suppose that V is symmetric, which we do in Lemma 2.3 and Theorems 2.4/2.5 below.

We are interested in writing the heat kernel for H_A using the method of images. Some group theoretic notation will be useful. $\mathcal{P}_\nu$ is the set of subsets of $\{1, \dots, \nu\}$ which forms a group under $(A, B) \mapsto A \triangle B$, the symmetric difference. The identity is $\emptyset$, the empty set. As a finite abelian group, $\mathcal{P}_\nu$ is its own dual. The character χ_A associated to $A \in \mathcal{P}_\nu$ acts by

$$\chi_A(B) = (-1)^{|A\cap B|}. \tag{9}$$

In particular, orthogonality of characters implies

Lemma 2.2.

$$\sum_{B\in\mathcal{P}_\nu} \chi_A(B)\chi_C(B) = 2^\nu \delta_{AC}.$$

Given $B \in \mathcal{P}_\nu$, define the reflection R_B acting on $\mathbb{R}^\nu$ by

$$R_B = \prod_{j\in B} \pi_j.$$

The method of images formula then says

Lemma 2.3. *If x, y are in the same orthant, then*

$$\exp(-tH_A)(x, y) = \sum_{B\in\mathcal{P}_\nu} \chi_B(A) \exp(-tH)(x, R_B y)$$

and the integral kernel is zero if x, y are in different orthants.

This immediately yields:

Theorem 2.4. *Let $C_t = \sum_{A\in\mathcal{P}_\nu} (-1)^{|A|} \exp(-tH_A)$. Then the integral kernel of C_t is*

$$C_t(x, y) = \begin{cases} 2^\nu \exp(-tH)(x, -y), & x, y \text{ in the same orthant} \\ 0, & x, y \text{ in different orthants.} \end{cases}$$

Proof. Let $B_0 = \{1, \dots, \nu\}$ so $R_{B_0} y = -y$ and $\chi_{B_0}(A) = (-1)^{|A|}$ so if x, y lie in the same orthant:

$$\begin{aligned} C_t(x,y) &= \sum_{A \in \mathcal{P}_\nu} \chi_{B_0}(A) \exp(-tH_A)(x,y) \\ &= \sum_{\substack{A \in \mathcal{P}_\nu \\ B \in \mathcal{P}_\nu}} \chi_{B_0}(A) \chi_B(A) \exp(-tH_A)(x, R_B y) \qquad \text{(by Lemma 2.3)} \\ &= 2^\nu \sum_{B \in \mathcal{P}_\nu} \delta_{B_0 B} \exp(-tH)(x, R_B y) \qquad \text{(by Lemma 2.2)} \\ &= 2^\nu \exp(-tH)(x, -y). \quad \square \end{aligned}$$

Theorem 2.5. *Let V be bounded below and $t > 0$. Then the operator C_t of Theorem 2.4 is a trace class opertor in $L^2(\mathbb{R}^\nu)$ and*

$$\operatorname{Tr}(C_t) = 2^\nu \int_{\mathbb{R}^\nu} \exp(-tH)(x, -x)\, d^\nu x.$$

Proof. Let $S_t = \exp(-tH)$. For $\alpha \in \tilde{\mathbb{Z}}^\nu \equiv \mathbb{Z}^\nu + (\frac{1}{2}, \dots, \frac{1}{2})$ let χ_α be the characteristic function of $\{x \mid |x_i - \alpha_i| < \frac{1}{2},\ \text{all } i\}$, and let P_α be the projection which is multiplication by χ_α. Let $\tilde{\mathbb{Z}}^\nu_+ = \{\alpha \in \tilde{\mathbb{Z}}^\nu \mid \alpha_i > 0\}$.

C_t is a direct sum of 2^ν operators, each unitarily equivalent to $\tilde{C}_t := C_t \restriction \{x \mid x_i > 0\}$. Let R_{B_0} be the reflection $x \to -x$. Then by Theorem 2.4:

$$\tilde{C}_t = 2^\nu \sum_{\alpha, \beta \in \tilde{\mathbb{Z}}^\nu_+} P_\alpha R_{B_0} S_t P_\beta.$$

By the lemma below, $P_\alpha R_{B_0} S_t P_\beta$ is trace class with trace norm bound by $C_1 \exp(-C_2|\alpha + \beta|)$ and trace given by the integral of the diagonal integral kernel. Since $\sum_{\alpha, \beta \in \tilde{\mathbb{Z}}^\nu_+} \exp(-C_2|\alpha + \beta|) < \infty$, the result follows. $\square$

Lemma 2.6. *In the notation of the last proof, $P_\alpha R_{B_0} S_t P_\beta$ is trace class with trace norm bounded by $C_1 \exp(-C_2|\alpha+\beta|)$ and trace given by the integral of the diagonal of the (continuous) integral kernel.*

Proof. $P_\alpha R_{B_0} S_t P_\beta = \sum_{\gamma \in \tilde{\mathbb{Z}}^\nu} R_{B_0}(P_{-\alpha} S_{t/2} P_\gamma)(P_\gamma S_{t/2} P_\beta)$. By a standard estimate (see, e.g., [9]):

$$|S_u(x,y)| \le C_{1,u} \exp(-C_{2,u}|x - y|)$$

(of course one can even have $|x - y|^2$ but we don't need that), so by integrating the square of the integral kernel:

$$\|P_\alpha S_{t/2} P_\gamma\|_2 \le C_3 \exp(-C_2|\alpha - \gamma|),$$

where $\|\cdot\|_2$ is the Hilbert-Schmidt norm. Summing over γ, we obtain the trace class result and bound since

$$\sum_{\gamma \in \tilde{\mathbb{Z}}^\nu} \exp(-C_2|\alpha + \gamma|) \exp(-C_2|\beta - \gamma|) \le C_5 \exp(-C_4|\alpha + \beta|).$$

Since the trace of a product of Hilbert-Schmidt operators is given by the integral of the diagonal integral kernel, we obtain the trace result. $\square$

§3. A Gaussian Process

In this section, we present a Feynman-Kac type formula for $\mathrm{Tr}(C_t)$ where C_t is the operator of Theorem 2.4. If V is bounded, (7) is an immediate consequence of this formula. For V unbounded (from above) at infinity, we will need an additional estimate on the Gaussian process, $\mathbf{L}(t)$, used in this formula and that estimate appears at the end of this section. (We shall employ the notation used in [8], i.e., $E(f) = \int_\Omega f\,d\mu$, $E(A) = \int_A d\mu = \mu(A)$, $E(f;A) = \int_A f\,d\mu$, etc., where $(\Omega, \mathcal{F}, \mu)$ denotes a probability space, $A \in \mathcal{F}$, $f : \Omega \to \mathbb{R}$ is $\mathcal{F}$-measurable.)

All Gaussian processes considered in this paper have mean zero and we will suppose that without explicitly saying it each time. Recall [8] that the Brownian bridge $\{\alpha(s)\}_{0\le s\le 1}$ is the Gaussian process with covariance:

$$\begin{aligned} E_\alpha(\alpha(s)\alpha(t)) &= \min(s,t)(1-\max(s,t)) \\ &= \frac{1}{2}(s+t-|s-t|) - st. \end{aligned} \tag{10}$$

If $b(s)$ is Brownian motion, then $\alpha(s) = b(s) - sb(1)$ is an explicit realization of the Brownian bridge. The ν-dimensional Brownian bridge is ν independent copies of $\alpha(s)$ thought of as a vector valued process and one still has for the ν-dimensional objects

$$\boldsymbol{\alpha}(s) = \mathbf{b}(s) - s\mathbf{b}(1). \tag{11}$$

Let $\mathbf{g}_{\mathbf{x},\mathbf{y}}(s) = s\mathbf{x} + (1-s)\mathbf{y}$ be the straight line from $\mathbf{x}$ to $\mathbf{y}$. Then, [8] shows that for any V bounded from below (and locally bounded from above, say), if $H = -\Delta + V$ in $L^2(\mathbb{R}^\nu)$,

$$\exp(-tH)(\mathbf{x},\mathbf{y}) = \exp(t\Delta)(\mathbf{x},\mathbf{y}) E_\alpha\biggl(\exp\biggl(-\int_0^t V\Bigl(\mathbf{g}_{\mathbf{x},\mathbf{y}}\Bigl(\frac{s}{t}\Bigr) + \sqrt{2t}\,\boldsymbol{\alpha}\Bigl(\frac{s}{t}\Bigr)\Bigr)\,ds\biggr)\biggr). \tag{12}$$

We have $\sqrt{2t}$ rather than the $\sqrt{t}$ on pg. 54 of [8] because we use $-\Delta$ rather than $-\frac{1}{2}\Delta$. Plugging (12) into Theorem 2.5 we find that

$$\mathrm{Tr}(C_t) = \int_{\mathbb{R}^\nu} d^\nu x N_t(\mathbf{x}) E_\alpha\biggl(\exp\biggl(-\int_0^t V\Bigl(\mathbf{g}_{\mathbf{x},-\mathbf{x}}\Bigl(\frac{s}{t}\Bigr) + \sqrt{2t}\,\boldsymbol{\alpha}\Bigl(\frac{s}{t}\Bigr)\Bigr)\,ds\biggr)\biggr),$$

where $N_t(\mathbf{x}) = 2^\nu \exp(t\Delta)(\mathbf{x},-\mathbf{x}) = 2^\nu \exp(t\Delta)(2\mathbf{x},0) \equiv \prod_{i=1}^\nu \tilde{N}_t(x_i)$. Notice that $\tilde{N}_t(x_i)$ is a Gaussian probability distribution with variance $\langle x_{t,i}^2\rangle = \frac{2t}{(2)^2} = \frac{t}{2} = \frac{1}{4}(\sqrt{2t})^2$, so if we let $x_{0,i}$ be a Gaussian variable of variance $\langle x_{0,i}^2\rangle = \frac{1}{4}$, then $x_{t,i} = \sqrt{2t}\,x_{0,i}$. Note that $g_{\mathbf{x},-\mathbf{x}}(\frac{s}{t}) = \sqrt{2t}\,\mathbf{x}_0(2(\frac{s}{t})-1)$.

This suggests we define a new process

$$\mathbf{L}(s) = \mathbf{x}_0(2s-1) + \boldsymbol{\alpha}(s), \qquad 0 \le s \le 1, \tag{13}$$

where the components of $\mathbf{x}_0$ are independent Gaussian variables with $\langle x_{0,i}^2\rangle = \frac{1}{4}$ and independent of $\boldsymbol{\alpha}$ so

$$\begin{aligned} E(\mathbf{L}_i(s)\mathbf{L}_j(w)) &= E_\alpha(\boldsymbol{\alpha}_i(s)\boldsymbol{\alpha}_j(w)) + \frac{\delta_{ij}}{4}(2s-1)(2w-1) \\ &= \delta_{ij}\left[\frac{1}{4} - \frac{1}{2}|s-w|\right]. \end{aligned} \tag{14}$$

We have thus proven that:

Theorem 3.1. *Let* $\mathbf{L}$ *be the Gaussian process with covariance* (14). *Then* (*with* C_t *given by Theorem* 2.4)*:*

$$\operatorname{Tr}(C_t) = E\left(\exp\left(-\int_0^t V\left(\sqrt{2t}\,\mathbf{L}\left(\frac{s}{t}\right)\right) ds\right)\right).$$

We need the following estimate on $\mathbf{L}$:

Theorem 3.2. $E\big(\{[\sup_{0\le s\le 1} |\mathbf{L}(s)|] \ge a\}\big) \le C_1 \exp(-C_2 a^2)$ *for some* $C_1, C_2 > 0$.

Proof. By the realizations (13) and (11), $\mathbf{L}(s) = \mathbf{b}(s) - s\mathbf{b}(1) + \mathbf{x}_0(2s-1)$ so

$$\sup_{0\le s\le 1} |\mathbf{L}(s)| \le |\mathbf{x}_0| + |\mathbf{b}(1)| + \sup_{0\le s\le 1} |\mathbf{b}(s)| \tag{15}$$

and for the $\sup_{0\le s\le 1} |\mathbf{L}(s)|$ to be larger than a, one or more of the three terms on the right side of (15) must be larger than $a/3$. Each has a Gaussian bound since $\mathbf{x}_0$ and $\mathbf{b}(1)$ are Gaussian and $\sup_{0\le s\le 1} |\mathbf{b}(s)|$ has a Levy inequality estimate (see [8], pp. 64 ff). □

Remarks. 1. Each component of $\mathbf{L}(t)$ is an independent copy of the one-dimensional $L(t)$. $L(t)$ is intimately related to the xi process, ω, we introduced in [2]; namely

$$\begin{aligned} L(t) &= \omega(t), & t &\le T_\omega \\ &= -\omega(t), & t &\ge T_\omega, \end{aligned}$$

where T_ω is the first time that $\omega(t) = 0$, that is, ω and L are related by reflection at a first hitting time. Theorem 3.2 is thus another proof of the estimate we proved on the xi process in [2].

2. The covariance (14) associated with $L(t)$ is just the zero energy Green's function for $-\frac{d^2}{dx^2}$ on $L^2([0,1])$ with antiperiodic boundary conditions, just as (10) is the Dirichlet Green's function. Notice that $L(1) = -L(0)$ is related to the antiperiodicity.

§4. The Main Result in Unbounded Space

Given Theorems 2.5, 3.1, and 3.2, the proof of (7) is easy following the methods of [2,8]:

Theorem 4.1. *Let V be bounded from below and continuous on $\mathbb{R}^\nu$. Let* $C_t = \sum\limits_{A\in\mathcal{P}_\nu} (-1)^{|A|}$ $\exp(-tH_A)$, $t>0$. *Then C_t is a trace class operator in $L^2(\mathbb{R}^\nu)$ and*

$$\operatorname{Tr}(C_t) = 1 - tV(0) + o(t) \qquad \text{as } t\downarrow 0.$$

Proof. As noted in Lemma 2.1, we can suppose that V is symmetric. By Theorems 2.5 and 3.1:

$$\begin{aligned}\operatorname{Tr}(C_t) &= E\left(\exp\left(-\int_0^t V\left(\sqrt{2t}\,L\left(\frac{s}{t}\right)\right)ds\right)\right)\\ &= T_1(V) + T_2(V),\end{aligned}$$

where

$$T_i(V) = E\left(\chi_{i,t}(L)\exp\left(-\int_0^t V\left(\sqrt{2t}\,L\left(\frac{s}{t}\right)\right)ds\right)\right)$$

and $\chi_{1,t}$ is the characteristic function of $\{L \mid \sup\limits_{0\le s\le 1}|L(s)| < t^{-1/3}\}$ and $\chi_{2,t} = 1-\chi_{1,t}$.

By Theorem 3.2, $|T_2(V)| \le C_1\exp(-t\inf|V(x)|)\exp(-C_2/t^{2/3}) = o(t)$ and $E(\chi_{1,t}(L))$ $= 1 + o(t)$, thus

$$\begin{aligned}\lim_{t\downarrow 0}(T_1(V)-1)/t &= \lim_{t\downarrow 0} E\left(\chi_{1,t}(L)t^{-1}\left\{\exp\left(-\int_0^t V\left(\sqrt{2t}\,L\left(\frac{s}{t}\right)\right)ds - 1\right\}\right)\right.\\ &= V(0)\end{aligned}$$

by continuity and dominated convergence (since V is bounded near 0). $\square$

Remark. Because we use path integral estimates, continuity of V is not needed. One only needs conditions that can be stated in terms of the Kato class K_ν defined as

$$K_\nu = \left\{V \mid \lim_{\beta\downarrow 0}\left[\sup_{x\in\mathbb{R}^\nu}\int_{|x-y|\le\beta} |x-y|^{-(\nu-2)}|V(y)|\,d^\nu y = 0\right]\right\}$$

(if $\nu=2$, $|x-y|^{-(\nu-2)}$ is replaced by $\ln(|x-y|^{-1})$) and in terms of the Stummel class $M_{2-\alpha,1}$ (see, e.g., [9]):

$$M_{2-\alpha,1} = \left\{V \mid \sup_{x\in\mathbb{R}^\nu}\int_{|x-y|\le 1} |x-y|^{-(\nu-2)-\alpha}|V(y)|\,d^\nu y < \infty\right\}.$$

By using the methods of [2], one can prove Theorem 4.1 if

(a) $\min(V, 0)$ is in the Kato class K_ν.
(b) V is in a local Stummel class $M_{2-\alpha,1}$ for some $\alpha > 0$ (i.e., $V\chi_R \in M_{2-\alpha,1}$ for all $R > 0$, where χ_R denotes the characteristic function of the ball $\{x \in \mathbb{R}^\nu \mid |x| \leq R\}$).
(c) 0 is a point of Lebesgue continuity for V for averaging over balls shrinking to zero.

Just as we could write the one-dimensional trace formula as either (5) or (6), in low dimension one can use the method of images to write C_t in alternate ways that avoid mixed boundary conditions. For example, in two dimensions, let H^D be what we called $H_{A=\{1,2\}}$ resp. $H^N = H_{A=\emptyset}$ correspond to Dirichlet resp. Neumann boundary conditions on both axes. Then by the method of images (i.e., Lemma 2.3):

$$e^{-tH^D}(x,x) + e^{-tH^N}(x,x) = 2e^{-tH}(x,x) + 2e^{-tH}(x,-x), \qquad x \in \mathbb{R}^2$$

so we have

Proposition 4.2. *In two dimensions*

$$\mathrm{Tr}(C_t) = 2\int_{\mathbb{R}^2} \big[e^{-tH^D} + e^{-tH^N} - 2e^{-tH}\big](x,x)\, d^2x.$$

Remark. Note we have not stated in the proposition that $[\dots]$ in the last integral is trace class because it is not in general. For example, if $V = 0$, it is not even Hilbert-Schmidt because of the contribution of the integral kernel $-2e^{-tH}(x,y)$ with $x = (u_1, v_1)$, $y = (-u_2, v_2)$, $0 < u_i < 1$, $0 < v_i < \infty$, $|v_1 - v_2| < 1$.

Remark. There are also results for Dirichlet conditions only. Explicitly, for $A \subset \{1, \dots, \nu\}$, let $\tilde{H}_{A;x}$ be the operator with Dirichlet boundary conditions on the planes $P_j^{(x)}$ with $j \in A$ but no conditions on the planes with $j \notin A$ (i.e., free boundary conditions, so, e.g., if $A = \emptyset$, the $\tilde{H}_{A;x}$ is just $-\triangle + V$). Then we can show that if

$$B_t = \sum_{A\subset\{1,\dots,\nu\}} (-1)^{|A|} \exp(-t\tilde{H}_{A;x})$$

has a continuous integral kernel, then

$$\int_{\mathbb{R}^\nu} B_t(y,y)\, d^\nu y = 2^{-\nu}[1 - tV(x) + o(t)].$$

This generalizes (5). We believe that B_t is always trace class but have only proven that if $V$is symmetric under reflection in each of the planes $P_j^{(x)}$.

§5. The Main Result in a Box

Our main goal here is to prove:

Theorem 5.1. *Let V be continuous on $[0,1]^\nu$. For $A \subset \{1,\dots,\nu\}$, let H_A be $-\Delta + V$ on $L^2([0,1]^\nu)$ with Dirichlet boundary condition on the hyperplanes with $x_j = 0$ or $x_j = 1$ and $j \in A$ and Neumann boundary condition on the hyperplanes with $x_j = 0$ or $x_j = 1$ and $j \notin A$. Let $\langle V \rangle$ be the average of V at the 2^ν corners of $[0,1]^\nu$. Then*

$$\sum_{A \subset \{1,\dots,\nu\}} (-1)^{|A|} \operatorname{Tr}(e^{-tH_A}) = 1 - t\langle V \rangle + o(t) \qquad \text{as } t \downarrow 0.$$

Remarks. 1. We take a unit cube for notational simplicity only. The result holds without change on $\mathop{\times}\limits_{i=1}^{\nu} [a_i, b_i]$. But rectangular symmetry is critical. It may be possible to extend the result to the unit cells for some other space groups with enough reflections.

2. If V is continuous and periodic with period one in each direction, then of course $\langle V \rangle = V(0)$.

3. All one needs is that V lies in the Kato class and suitable Lebesgue continuity of V at each corner.

In the group theoretical part of the proof we gave of (7), the key was that $\mathcal{P}_\nu$ was the group generated by the π_j's. Let ρ_j be the reflection in $x_j = 1$, that is,

$$\begin{aligned} [\rho_j(x)]_i &= x_i, && i = j \\ &= 2 - x_j, && i \neq j. \end{aligned}$$

Let $\mathcal{G}_\nu$ be the group of actions on $\mathbb{R}^\nu$ generated by the π_j's and ρ_j's. Then it is easy to see that V has a unique extension to $\mathbb{R}^\nu$ which is $\mathcal{G}_\nu$ invariant and this extension, which we'll also call V, is continuous on $\mathbb{R}^\nu$. Let $H = -\Delta + V$ on $L^2(\mathbb{R}^\nu)$.

$\mathcal{G}_\nu$ is a semidirect product $2\mathbb{Z}^\nu \circledS \mathcal{P}_\nu$, so every $G \in \mathcal{G}_\nu$ can be written as $G = (\mathbf{a}, B)$ where $\frac{1}{2}\mathbf{a} \in \mathbb{Z}^\nu$ and G acts by

$$Gx = R_B x + a.$$

Define for $A \in \mathcal{P}^\nu$,

$$\chi_A(G) = (-1)^{|A \cap B|}.$$

Then the method of images formula for e^{-tH_A} is:

Proposition 5.2. *If $x, y \in [0,1]^\nu$, $A \in \mathcal{P}_\nu$, then*

$$e^{-tH_A}(x,y) = \sum_{G \in \mathcal{G}_\nu} \chi_A(G) e^{-tH}(x, Gy).$$

As in §2, let R_{B_0} be the inversion in 0, that is, $R_{B_0}x = -x$. Then Lemma 2.2 implies

$$\sum_{A \in \mathcal{P}_\nu} (-1)^{|A|} \chi_A(G) = \begin{cases} 2^\nu & \text{if } G = (\mathbf{a}, B_0) \\ 0 & \text{if } G = (\mathbf{a}, B) \text{ with } B \neq B_0 \end{cases}$$

and we conclude that

Proposition 5.3.

$$\sum_{A\in\mathcal{P}_\nu} (-1)^{|A|}\operatorname{Tr}(e^{-tH_A}) = \sum_{a\in\mathbb{Z}^\nu} M(a,t),$$

where

$$M(a,t) \equiv 2^\nu \int\limits_{[0,1]^\nu} e^{-tH}(x, 2a-x)\, d^\nu x.$$

With these preliminaries we are ready for the

Proof of Theorem 5.1. Let Q be the set of 2^ν corners of $[0,1]^\nu$ as points in $\mathbb{Z}^\nu$. If $a \in \mathbb{Z}^\nu \backslash Q$, then

$$\min_{x\in[0,1]^\nu} \operatorname{dist}(x, 2a-x) = 2 \min_{x\in[0,1]^\nu} \|x-a\| \geq 2. \tag{16}$$

Since (see, e.g., [9])

$$|e^{-tH}(x,y)| \leq C_1 \exp(-C_2(x-y)^2/t), \tag{17}$$

(16) implies

$$\sum_{a\in\mathbb{Z}^\nu\backslash Q} M(a,t) = O(e^{-c/t})$$

so by Proposition 5.3, it suffices to prove that for $a \in Q$:

$$M(a,t) = 2^{-\nu}[1 - V(a)t + o(t)]. \tag{18}$$

By translation and reflection symmetry, we need only prove (18) for $a = 0$. But by (17):

$$\begin{aligned} M(0,t) &= 2^\nu \int\limits_{x_i\geq 0} e^{-tH}(x,-x)\, d^\nu x + O(e^{-c/t}) \\ &= \int\limits_{\mathbb{R}^\nu} e^{-tH}(x,-x)\, d^\nu x + O(e^{-c/t}) \end{aligned}$$

so (18) is precisely (7) given Theorem 2.5. $\square$

Remark. Because V is bounded, we do not need the estimate in Theorem 3.2 to prove Theorem 5.1.

The proof of Theorem 5.1 shows:

Theorem 5.4. *Let V be continuous on $[0,1]^\nu$. For $A \subset \{1,\dots,\nu\}$, let $\tilde{H}_A$ be $-\Delta + V$ on $L^2([0,1]^\nu)$ with Dirichlet boundary conditions on the hyperplanes with $x_j = 0$ for $j \in A$ and Neumann boundary conditions on the hyperplanes with $x_j = 0$ for $j \notin A$ or $x_k = 1$ for all $k \in \{1,\dots,\nu\}$. Then*

$$\sum_{A\subset\{1,\dots,\nu\}} (-1)^{|A|}\operatorname{Tr}(e^{-t\tilde{H}_A}) = 2^{-\nu}[1 - tV(0) + o(t)] \qquad \text{as } t\downarrow 0.$$

Proof. We still use the same group $\mathcal{G}_\nu$. Define with $G = (\mathbf{a}, B) \in \mathcal{G}_\nu$

$$\tilde{\chi}_A(G) = (-1)^{|A \cap B|}(-1)^{(1/2)\sum_{j\in A}|a_j|}.$$

$\mathcal{G}_\nu$ is generated by $\{\pi_j\} \cup \{\rho_j\}$ and

$$\begin{aligned} &\tilde{\chi}_A(\pi_j) = -1 \quad (\text{resp. } 1) && \text{for } j \in A \quad (\text{resp. } j \notin A) \\ &\tilde{\chi}_A(\rho_j) = 1 && \text{for all } j = 1, \dots, \nu \end{aligned}$$

and $\tilde{\chi}$ is a character. Hence we have our method of images formula

$$e^{-t\tilde{H}_A}(x,y) = \sum_{G\in\mathcal{G}_\nu} \tilde{\chi}_A(G)\, e^{-tH}(x, Gy)$$

with H associated to the G invariant extension of V as in Proposition 5.2.

Note that for $G \in \mathcal{G}_\nu$ fixed, $A \mapsto \tilde{\chi}_A(G)$ is a character on $\mathcal{P}_\nu$. By the orthogonality of characters

$$\sum_{A\in\mathcal{P}_\nu} (-1)^{|A|}\tilde{\chi}_A(G) = \begin{cases} 2^\nu & \text{if } \tilde{\chi}_A(G) \equiv (-1)^A \\ 0 & \text{if } \tilde{\chi}_A(G) \not\equiv (-1)^{|A|}. \end{cases}$$

But $\tilde{\chi}_A(G) \equiv (-1)^{|A|}$ if and only if $G = (\mathbf{a}, B)$ with $B = B_0$ and each $\frac{1}{2}a_i$ is even. Thus, as in the proof of Proposition 5.3,

$$\sum_{A\in\mathcal{P}_\nu} (-1)^{|A|}\mathrm{Tr}(e^{-t\tilde{H}_A}) = \sum_{a\in 2\mathbb{Z}^\nu} M(a,t)$$

with the same M's. This completes the proof. $\square$

Our next result, an analog of Proposition 4.2, is an abelianized version of a formula that Lax [5] derived formally in two dimensions:

Theorem 5.5. *Let V be a continuous periodic function on $\mathbb{R}^2$ with $V(x_1+n_1, x_2+n_2) = V(x_1,x_2)$ for $\mathbf{n} = (n_1,n_2) \in \mathbb{Z}^2$. Let $H_P, H_A, H_{AP}, H_{PA}, H_N, H_D$ be the operators on $L^2([0,1]^2)$ with periodic, antiperiodic, AP, PA, Neumann, and Dirichlet boundary conditions where AP (resp. PA) means antiperiodic in the x_1 (resp. x_2) direction and periodic in the x_2 (resp. x_1) direction. Then*

$$\begin{aligned} \mathrm{Tr}(e^{-tH_P} + e^{-tH_A} + e^{-tH_{PA}} + e^{-tH_{AP}} - 2e^{-tH_N} - 2e^{-tH_D}) \\ = -1 + tV(0) + o(t) \qquad \text{as } t \downarrow 0. \end{aligned} \tag{19}$$

Proof. Let $\tilde{V}$ be the extension of V given by reflection, and $\tilde{H} = -\Delta + \tilde{V}$. By the method of images as above,

$$2\mathrm{Tr}(e^{-tH_N} + e^{-tH_D}) = \sum_{a\in\mathbb{Z}^2} \tilde{M}(a,t) + \sum_{a\in\mathbb{Z}^2} \tilde{N}(a,t),$$

where $\tilde{M}$ is defined in Proposition 5.3 (with H replaced by $\tilde{H}$) and

$$\tilde{N}(a,t) = 4 \int\limits_{[0,1]^2} e^{-t\tilde{H}}(x, x+2a)\, d^2x.$$

By (17) and (18)

$$2\mathrm{Tr}(e^{-tH_N} + e^{-tH_D}) = 1 - tV(0) + \tilde{N}(0,t) + O(e^{-c/t}).$$

Now let $H = -\Delta + V$. Then

$$4\mathrm{Tr}(e^{-tH_P}) = \sum_{a\in\mathbb{Z}^2} N\left(\frac{1}{2}a, t\right)$$

with

$$N\left(\frac{1}{2}a, t\right) = 4 \int\limits_{[0,1]^2} e^{-tH}(x, x+a)\, d^2x.$$

By (17) again

$$4\mathrm{Tr}(e^{-tH_P}) = N(0,t) + O(e^{-c/t}).$$

Similar formulae show that

$$4\mathrm{Tr}(e^{-tH_A}) = N(0,t) + O(e^{-c/t})$$

and for H_{AP} and H_{PA}. Thus

$$\text{LHS of (19)} = -1 + tV(0) + o(t) + [N(0,t) - \tilde{N}(0,t)]$$

and (19) follows from the following assertion (20):

$$N(0,t) - \tilde{N}(0,t) = o(t). \tag{20}$$

The proof of (20) is a little subtle because the integral kernel $e^{-tH}(x,x)$ is $O(t^{-1})$ as $t \downarrow 0$ in two dimensions. In terms of a path integral expansion, only points $O(t^{1/2})$ from the border contribute. Thus to get an $o(t)$ error, we must have complete cancellation of the $O(t)$ terms in the expansion of the exponentials in the path integral.

So let $\mathbf{w}_t(s)$ be $\mathbf{x}+\sqrt{2t}\,\boldsymbol{\alpha}(\frac{s}{t})$ where $\boldsymbol{\alpha}$ is the Brownian bridge and x is independent of $\boldsymbol{\alpha}$ and uniformly distributed on $[0,1]^2$. Define

$$g(\mathbf{w}_t, t) := \int\limits_0^t V(\mathbf{w}_t(s))\, ds$$

and $\tilde{g}$ with V replaced by $\tilde{V}$ and let

$$f(y) = e^{-y} - 1 + y.$$

Then

$$\begin{aligned} N(0,t) - \tilde{N}(0,t) &= (4\pi t)^{-1} E(e^{-g} - e^{-\tilde{g}}) \\ &\equiv A + B, \end{aligned}$$

where

$$\begin{aligned} A &= -(4\pi t)^{-1} E(g - \tilde{g}), \\ B &= (4\pi t)^{-1} E(f(g) - f(\tilde{g})). \end{aligned}$$

We'll prove that $A = 0$ and $B = O(t^{3/2-\epsilon})$, $\epsilon > 0$.

That $B = O(t^{3/2-\epsilon})$ follows by noting first that $|f(y)| \leq Cy^2$ on $[-1,1]$ and that $|g(\mathbf{w}_t, t)| \leq Ct$ uniformly in $\mathbf{w}$ so $|f(g) - f(\tilde{g})| \leq Ct^2$ uniformly in $\mathbf{w}$. On the other hand, if $\operatorname{dist}(x, \partial[0,1]^2) \geq t^{1/2-\epsilon}$, $\operatorname{Prob}(x + \sqrt{2t}\,\alpha(\frac{s}{t}) \notin [0,1]^2$ for some $s) \leq \exp(-C/t^{2\epsilon})$, so, since $f(g) = f(\tilde{g})$ if $\mathbf{w}_t(s) \in [0,1]^2$ for all s, we have

$$E(|f(g) - f(\tilde{g})|) \leq O(\exp(-t^{-2\epsilon})) + Ct^2 t^{1/2-\epsilon}$$

and we conclude that $B = O(t^{3/2-\epsilon})$ as required.

$A = 0$ because of a cancellation. Let $\rho_t(x)$ be the probability density of $\mathbf{w}_t(s)$ where s is uniformly distributed in $[0,1]$. Then

$$A = -(4\pi)^{-1} \int_{\mathbb{R}^2} \rho_t(x)[V(x) - \tilde{V}(x)]\, d^2x. \tag{21}$$

For each $\alpha \in \mathbb{Z}^2$, let $\square_\alpha$ be the square centered at $(\frac{1}{2}, \frac{1}{2}) + \alpha$. There is a symmetry $S_\alpha : \square_\alpha \to \square_{-\alpha}$ so that $V \circ S_\alpha = \tilde{V}$ and $\rho_t \circ S_\alpha = \rho_t$ so that the contribution of V over $\square_\alpha$ in (21) cancels the contribution of $\tilde{V}$ over $\square_{-\alpha}$. $\square$

A different kind of a two-dimensional trace formula for $V(x)$ by comparing heat kernels for $H = -\triangle + V$ and $H_o = -\triangle$ with Dirichlet boundary conditions on a rectangular box was recently studied in [7].

§6. Sums Without Abelian Summation

An interesting issue on which we haven't much to report is the extent to which a formula like (2) holds. We note:

Theorem 6.1. *In the context of Theorem* 5.1*, let* $\{E_n\}_{n=0}^\infty$ *be a listing of all the eigenvalues of* $\{H_A \mid |A| \text{ is even}\}$ *and* $\{\tilde{E}_n\}_{n=1}^\infty$ *for* $\{H_A \mid |A| \text{ is odd}\}$ *ordered so* $E_n \leq E_{n+1}; \tilde{E}_n \leq \tilde{E}_{n+1}$. *Suppose that*

$$\sum_{n=1}^\infty |E_n - \tilde{E}_n| < \infty. \tag{22}$$

Then

$$\langle V \rangle = E_0 + \sum_{n=1}^\infty (E_n - \tilde{E}_n).$$

Remark. Note that the counting of E_n starts at 0, but for $\tilde{E}_n$ at 1.

Proof. Theorem 5.1 says that

$$\langle V \rangle = \lim_{t \downarrow 0} \left[t^{-1}(1 - e^{-tE_0}) + \sum_{n=1}^{\infty} t^{-1}(e^{-t\tilde{E}_n} - e^{-tE_n}) \right].$$

If $0 \leq t \leq 1$, then

$$|e^{-ta} - e^{-tb}| \leq [e^{-t \min(a,b)} + 1]|a - b|$$

and

$$\lim_{t \downarrow 0} t^{-1}(e^{-ta} - e^{-tb}) = b - a$$

so the result follows by dominated convergence. $\square$

When $V = 0$, it is easy to see that $E_n = \tilde{E}_n$, $n \in \mathbb{N}$ so (22) holds. It remains to be seen if one can prove it for sufficiently smooth V's.

Acknowledgments. We would like to thank Peter Lax for telling us of his work prior to publication. F.G. is indebted to M. Aschbacher and G. Neugebauer for the hospitality at Caltech where some of this work was done. F.G. and H.H. were also supported in part by the Norwegian Research Council for Science and the Humanities (NAVF).

References

[1] H. Flaschka, *On the inverse problem for Hill's operator*, Arch. Rat. Mech. Anal. **59** (1975), 293–309.

[2] F. Gesztesy, H. Holden, B. Simon, and Z. Zhao, *Higher order trace relations for Schrö-dinger operators*, to be submitted to Commun. Pure Appl. Math.

[3] F. Gesztesy and B. Simon, *The xi function*, to be submitted to Ann. Math.

[4] H. Hochstadt, *On the determination of a Hill's equation from its spectrum*, Arch. Rat. Mech. Anal. **19** (1965), 353–362.

[5] P. Lax, *The trace formula for the Schrödinger operator*, to appear in Commun. Pure Appl. Math.

[6] H.P. McKean and P. van Moerbeke, *The spectrum of Hill's equation*, Invent. Math. **30** (1975), 217–274.

[7] V.G. Papanicolaou, *Trace formulas and the behavior of large eigenvalues*, to appear in SIAM J. Math. Anal.

[8] B. Simon, *Functional Integration and Quantum Physics*, Academic Press, New York, 1979.

[9] B. Simon, *Schrödinger semigroups*, Bull. Amer. Math. Soc. **7** (1982), 447–526.