A Trace Formula for Discrete Schrödinger Operators

By

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Abstract

We discuss two types of trace formula which arise from the inverse spectral problem for discrete Schrödinger operators as $L = -\Delta + V(x)$ where $V$ is a bounded potential. One is the relationship between a potential and spectral data, and another is the one between the green function of $L$ and periodic orbits of a state space.

§ 1. Introduction

The trace of the difference of two operators $L = -\Delta + V$ on $L^2(\mathbb{R}^1)$ and $L_{\alpha}$ that is imposed the Dirichlet condition at $x = \mathbb{R}^1$ has a relation

$$\text{Tr} (L - L_{\alpha}) = V(\alpha) = \lambda_0 + \sum_{j=1}^{\infty} \left( \lambda_{2j} + \lambda_{2j-1} - 2\mu_j \right)$$

for a periodic potential $V$, where $\{ \lambda_j \}$ is the collection of all eigenvalues with periodic and anti-periodic boundary conditions, and $\{ \mu_j \}$ is the collection of eigenvalues of certain Dirichlet Laplacian. It is the well known formula in Hill’s theory for periodic Schrödinger operators. In [2], it has been extended to the class which is called reflectionless potential containing periodic potential. In [4], they studied systematically trace formulas by using the scattering quantity which is called the Krein’s spectral shift function. We will show that similar results as these hold for a discrete Schrödinger operator $L$ on countable set and $L_A$ that is imposed the Dirichlet condition at a finite set $A$, that is.

**Theorem 1.1.** Let $G$ be a countable set and let $\Delta_G$ be a Laplacian on $G$. Let $V$ be a real-valued bounded function. Further, let $L = -\Delta_G + V$ and $L_A$ be imposed the Dirichlet condition on a finite set $A$. Then

$$\frac{1}{|A|} \text{Tr} (L - L_A) = \frac{1}{|A|} \sum_{\alpha \in A} V(\alpha) = \lambda_0 - 1 - \int_{\lambda_0}^{\lambda_\infty} \theta_A(\lambda) d\lambda$$

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where $\theta_A(\lambda)$ is a generalized Krein's spectral shift function.

Especially, if $G$ is $\mathbb{Z}^1$ and $A$ is a singleton $\{a\}$, then we can explicitly calculate of $\theta_A(\lambda)$, and the almost same relation as (1.1) holds.

In the area of quantum chaos, M. C. Gutzwiller has proposed the so-called Gutzwiller's trace formula [5]. It is the formula which connects the energy level (the spectrum of Schrödinger operators) with the classical periodic orbits. We will show that $\text{Tr}(G_2 - G_A^4)$ can be expanded by the periodic orbits on $A$ where $G_2$ (resp. $G_A^4$) is the resolvent of the operator $L$ (resp. $L_A$).

**Theorem 1.2.** There exists $\tilde{\lambda} \in \mathbb{R}$ such that for any $\lambda < \tilde{\lambda}$

$$\sum_{x \in G} (g_A(x, x) - g_A^4(x, x)) = \sum_{a \in A} \frac{d}{d\lambda} \log g_A(a, a)$$

$$+ \sum_{\gamma \in \Gamma} \frac{dS_\gamma(\lambda)}{d\lambda} \sum_{n \geq 1} \exp(-nS_\gamma(\lambda) - n\pi i L_\gamma)$$

where $\Gamma$ is the set of all prime periodic orbits, $L_\gamma$ is the period of $\gamma$ and $S_\gamma(\lambda)$ is the length of a periodic orbit $\gamma$ with respect to the distance $d_\gamma$ defined by (4.1).

It is thought as a discrete and heat version of the Gutzwiller's trace formula.

§ 2. A Trace Formula for the Inverse Spectral Problem

Let $G$ be a countable set and $P = \{p(x, y)\}_{x, y \in G}$ a transition probability. We assume that the transition probability is (1) $m$-symmetric, (2) irreducible and (3) simple, i.e., (1) there exists a positive real-valued function $m(x)$ on $G$ such that

$$m(x)p(x, y) = m(y)p(y, x)$$

for any $x, y \in G$, (2) for any $x, y \in G$ there exists a positive integer $N$ such that

$$p^N(x, y) > 0$$

and (3) $p(x, x) = 0$. ((3) is not essential but, for simplicity, we assume it.) Let $l^2(G, m)$ be an $l^2$-space with respect to the inner product given by

$$\langle f, g \rangle = \sum_{x \in G} m(x)f(x)g(x).$$

We define a discrete Laplacian on $l^2(G, m)$ as follows: for each $x \in G$.

$$\Delta_G \phi(x) = \sum_{r \in G} p(x, r) \phi(r) - \phi(x).$$

Let $V$ be a real-valued bounded function and we define a discrete Schrödinger operator by
Let \( A \subset G \) be a finite subset of \( G \). We consider two problems for our operator, i.e., one is
\[
L \phi (x) = \lambda \phi (x) \quad x \in G
\]
and the other is
\[
\begin{cases}
L_A \phi (x) = L \phi (x) = \lambda \phi (x) & x \in G \setminus A \\
L_A \phi (a) = 0 & a \in A,
\end{cases}
\]
and their domains are \( D(L) = l^2 (G, m) \) and \( D(L_A) = \{ f \in l^2 (G, m) ; f(a) = 0 \text{ for any } a \in A \} \). We denote the fundamental solutions of the associated heat equations by \( p^y(t, x, y) \) and \( p^A(t, x, y) \), respectively, and the associated green functions, that is, the integral kernels of \( (L - \lambda)^{-1} \) and \( (L_A - \lambda)^{-1} \) by \( g_t(x, y) \) and \( g^A_t(x, y) \), respectively. Remark that in general our heat kernels and green functions are not symmetric functions.

From now on, we assume that there exists a positive integer \( M \) such that
\[
\sup_{x \in G} \{ r \in G ; p(x, r) > 0 \} \leq M
\]
where \( |K| \) is the cardinality of a set \( K \). We can regard \( G \) as an infinite graph; then the assumption (2.1) means that the maximum degree is bounded.

To show our trace formula we calculate the trace \( \sum_{x \in G} (p^y(t, x, x) - p^A(t, x, x)) \) in two different ways. We use the following lemma for the first half of the trace formula.

**Lemma 2.1.** Let \( \{w_t, P_x\} \) be a continuous time random walk with the generator \( \Delta_G \), and \( T_A \) the first hitting time to the set \( A \). Then, as \( t \to 0 \),
\[
E_x[\delta_x (w_t)] = 1 - t + O(t^2)
\]
and
\[
\sum_{x \in G \setminus A} E_x[\delta_x (w_t) ; T_A \leq t] = O(t^2)
\]
where \( \delta_x(\cdot) \) is the indicator function of \( x \in G \).

**Proof.** Firstly, since \( \Delta_G \) is the generator of \( w_t \) and is bounded, we have
\[
E_x[\delta_x (w_t)] = \sum_{n \geq 0} \frac{t^n}{n!} \Delta_G^n \delta_x(a) = 1 + t (\Delta_G \delta_x) (a) + O(t^2) = 1 - t + O(t^2)
\]
as \( t \to 0 \).

Secondly, we define a metric on \( G \) as follows: for any \( x, y \in G \)
Put $M \geq 1$ as the assumption (2.1). Then it is obvious that the cardinality of a set $\{x \in G; d(x, A) = n\}$ is less than $|A| M^n$. Then we obtain
\[
\sum_{x \in G \setminus A} E_x[\delta_x(w_t); T_A \leq t] = \sum_{n \geq 1} \sum_{x \in G \setminus A} E_x[\delta_x(w_t); T_A \leq t]
\]
\[
\leq \sum_{n \geq 1} |A| M^n P_x[w \text{ has at least } 2n \text{ jumps up to time } t]
\]
\[
= \sum_{n \geq 1} |A| M^n \sum_{k \geq 2n} \frac{e^{-t} t^k}{k!} \leq \sum_{n \geq 1} |A| M^n t^{2n} \leq Ct^2 \quad \text{as } t \to 0.
\]
Here we used the fact that the number of jumps of the random walk up to time $t$ obeys the Poisson law with mean 1.

Now we show the first half of the trace formula.

**Proposition 2.2.** Let $V(x)$ be a real-valued bounded function on $G$. Then,
\[
\sum_{x \in G} (p^n V(t, x, x) - p^n V(t, x, x)) = |A| - t \left( \sum_{a \in A} V(a) + |A| \right) + O(t^2) \quad \text{as } t \to 0
\]
where $|A|$ is the cardinality of the set $A$.

**Proof.** By the Feynman-Kac formula, we have
\[
p^n V(t, x, x) = E_x[e^{-\int_0^t V(w_s) ds} (1 - \chi_{\{T_A > t\}}) \delta_x(w_t)]
\]
where $\chi_{\{T_A > t\}}$ is the indicator function of a set $\{T_A > t\}$. We consider the trace of the difference of two heat kernels
\[
\sum_{x \in G} (p^n V(t, x, x) - p^n V(t, x, x))
\]
\[
= \sum_{x \in G} E_x[e^{-\int_0^t V(w_s) ds} (1 - \chi_{\{T_A > t\}}) \delta_x(w_t)]
\]
\[
= \sum_{x \in G} \sum_{n \geq 0} \frac{(-1)^n}{n!} E_x \left[ \int_0^t V(w_s) ds \right]^n (1 - \chi_{\{T_A > t\}}) \delta_x(w_t) \right].
\]
For $n = 0$, by using Lemma 2.1 we have
\[
\sum_{x \in G} E_x[(1 - \chi_{\{T_A > t\}}) \delta_x(w_t)]
\]
\[
= \sum_{a \in A} E_a[\delta_a(w_t)] + \sum_{x \in G \setminus A} E_x[\delta_x(w_t); T_A \leq t]
\]
\[
= |A| (1 - t) + O(t^2) \quad \text{as } t \to 0.
\]
For $n = 1$, we have
where \( p^0(t, x, y) \) and \( p^\lambda(t, x, y) \) are the heat kernels for the case that the potential \( V \) is identically zero. Using the semigroup property, we have

\[
\sum_{x \in \mathbb{G}} E_x \left[ \left( \int_0^t V(w_s) \, ds \right) (1 - \chi_{\{T_s > t\}}) \, \delta_x(w_t) \right]
\]

\[
= \int_0^t ds \sum_{x \in \mathbb{G}} \sum_{y \in \mathbb{G}} (p^0(s, x, y) \, V(y) \, p^0(t-s, y, x) - p^\lambda(s, x, y) \, V(y) \, p^\lambda(t-s, y, x))
\]

Last we estimate the term for \( n \geq 2 \).

\[
\left| \sum_{n \geq 2} \frac{(-1)^n}{n!} \sum_{x \in \mathbb{G}} E_x \left[ \left( \int_0^t V(w_s) \, ds \right)^n (1 - \chi_{\{T_s > t\}}) \, \delta_x(w_t) \right] \right|
\]

\[
\leq \sum_{n \geq 2} \frac{t^n}{n!} \| V \|_{L^\infty} \sum_{x \in \mathbb{G}} E_x \left[ \left( 1 - \chi_{\{T_s > t\}} \right) \, \delta_x(w_t) \right]
\]

\[
\leq C t^2.
\]

Then, we have

\[
\sum_{x \in \mathbb{G}} (p^\lambda(t, x, x) - p^\lambda(t, x, x)) = |A| - t \left( \sum_{a \in A} V(a) + |A| \right) + O(t^2) \quad \text{as } t \to 0.
\]

Next we will calculate the difference of two green functions for the second half of the trace formula. Before doing that, we prepare a lemma.

**Lemma 2.3.** Let \( G^\lambda \) be a \( |A| \times |A| \) matrix with the elements \( (G^\lambda)_{a,b} = g^\lambda(a, b) \) for \( a, b \in A \). Then \( \det G^\lambda \) is holomorphic in \( \lambda \in \mathbb{C} \setminus \sigma(L) \). Moreover, for \( \lambda \in \mathbb{C} \setminus [\lambda_0, \lambda_\omega] \), the determinant \( \det G^\lambda \) is non-zero, where \( \sigma(L) \) is the spectral set of the operator \( L \), \( \lambda_0 = \inf \sigma(L) \) and \( \lambda_\omega = \sup \sigma(L) \).

**Proof.** Note that \( g^\lambda(x, y) \) is holomorphic in \( \lambda \in \mathbb{C} \setminus \sigma(L) \). It is obvious by the definition of the determinant that \( \det G^\lambda \) is also holomorphic in \( \lambda \in \mathbb{C} \setminus \sigma(L) \).
where \( \{e_x\}_{x \in \mathcal{G}} \) is an orthonormal basis of \( L^2(\mathcal{G}, m) \) such that
\[
e_x(y) = \begin{cases} m(x)^{-1/2} & \text{if } y = x, \\ 0 & \text{otherwise}, \end{cases}
\]
and \( E(\xi) \) is the resolution of the identity for the operator \( L \). Let \( f_0 \) be an \( |A| \)-dimensional vector such that \( \|f_0\|_A = 1 \), where \( \langle \cdot, \cdot \rangle_A \) is the inner product of \( L^2(\mathcal{A}, m) \). Let \( f \in L^2(\mathcal{G}, m) \) be the extension of \( f_0 \) such that \( \text{supp } f \subset A \), \( f(a) = f_0(a) \) for any \( a \in A \) and \( \|f\| = 1 \). Then we have
\[
\langle f_0, G_{\lambda} f_0 \rangle_A = \langle f, G_{\lambda} f \rangle = \int_{\sigma(L)} \frac{1}{\xi - \lambda} d\mu_\lambda(\xi)
\]
where \( d\mu_\lambda(\xi) = d\|E(\xi)f\|^2 \). We will estimate \( |\langle f, G_{\lambda} f \rangle| \) from below. Firstly, in the case that \( |\text{Im } \lambda| > 0 \), for any \( f \in L^2(\mathcal{G}, m) \), we have
\[
|\langle f, G_{\lambda} f \rangle| \geq \left| \int_{\sigma(L)} \frac{\text{Im } \lambda}{|\xi - \lambda|^2} d\mu_\lambda(\xi) \right|
\]
(2.5)
\[
\geq \frac{|\text{Im } \lambda|}{\max_{\xi \in \sigma(L)} |\xi - \lambda|^2}.
\]
Secondly, when \( \lambda \in \mathbb{R} \setminus [\lambda_0, \lambda_\infty] \), we have
\[
|\langle f, G_{\lambda} f \rangle| \geq \frac{1}{\max(|\lambda - \lambda_0|, |\lambda - \lambda_\infty|)}.
\]
In both cases, there exists a positive constant \( C(\lambda) \) depending only on \( \lambda \) such that \( |\langle G_{\lambda} f, f \rangle| \geq C(\lambda) > 0 \). Then, for any \( \lambda \in \mathbb{C} \setminus [\lambda_0, \lambda_\infty] \), \( \det G_\lambda \neq 0 \).

Remark 2.4. For \( \lambda \in [\lambda_0, \lambda_\infty] \cap \sigma(L)^c \), the determinant \( \det G_\lambda \) may vanish.

Lemma 2.5. \( \lambda \in \mathbb{C} \setminus [\lambda_0, \lambda_\infty] \). Then for any \( x, y \in \mathcal{G} \)
\[
g_{\lambda}(x, y) = g_{\lambda}^*(x, y) = \sum_{a \in A} g_{\lambda}(x, a) (G_{\lambda})^{-1} g_{\lambda}(a, y)
\]
where \( (G_{\lambda})^{-1} \) acts on the first variable.

Proof. Let \( F_\lambda(t) = F_\lambda(t, w) = \int_0^t (\lambda + V(w_t)) dt \). If \( \lambda < \inf_{x \in \mathcal{G}} V(x) \), \( F_\lambda(t) \)
\[
\geq 0, \text{ and so } F_\lambda(\infty) = \infty. \text{ For any } \lambda < \inf_{x \in \mathcal{G}} V(x) \text{, by the strong Markov property, we have}
\]
\[
g_{\lambda}(x, y) = E_x \left[ \int_0^\infty e^{-F_\lambda(t)} \delta_y(w_t) dt \right]
\]
where \((S_tw)_t = w_{t+s}\). We put 
\[ f_{x,}\lambda(a) = e^{-F_{\xi}(\lambda)}(x, a)\] for each \(a \in A\). Then,
\[ g_\lambda(x, y) - g_\lambda^A(x, y) = \sum_{a \in A} g_\lambda(a, y) \mu_{x, \lambda}(a).\]

Next, in the same way as above, we have
\[ g_\lambda(x, a) = \sum_{b \in A} g_\lambda(b, a) \mu_{x, \lambda}(b) \]
for each \(x \in G\) and \(a \in A\).

By Lemma 2.3, there exists an inverse matrix of \(G_\lambda^A\). Then we have
\[ \sum_{a \in A} g_\lambda(x, a) (G_\lambda^A)^{-1} g_\lambda(a, y) \]
\[ = \sum_{a \in A} \sum_{b \in A} g_\lambda(b, a) \mu_{x, \lambda}(b) (G_\lambda^A)^{-1} g_\lambda(a, y) \]
\[ = \sum_{b \in A} \mu_{x, \lambda}(b) \sum_{a \in A} g_\lambda(b, a) (G_\lambda^A)^{-1} g_\lambda(a, y) \]
\[ = \sum_{b \in A} \mu_{x, \lambda}(b) g_\lambda(b, y) = g_\lambda(x, y) - g_\lambda^A(x, y).\]

The lemma is obtained by analytic continuation.

**Proposition 2.6.** Let \(\lambda \in \mathbb{C} \setminus [\lambda_0, \lambda_\infty]\). Then
\[ (2.7) \quad \sum_{x \in G} (g_\lambda(x, x) - g_\lambda^A(x, x)) = \frac{d}{d\lambda} \log \det G_\lambda^A.\]

**Proof.** Since \((G_\lambda^A)^{-1}\) is a linear operator, taking summation over \(x \in G\), we have
\[ \sum_{x \in G} (g_\lambda(x, x) - g_\lambda^A(x, x)) = \sum_{x \in G} \sum_{a \in A} g_\lambda(x, a) (G_\lambda^A)^{-1} g_\lambda(a, x) \]
\[ = \sum_{a \in A} (G_\lambda^A)^{-1} \frac{d}{d\lambda} G_\lambda^A(a, a) = \text{Tr} \left( (G_\lambda^A)^{-1} \frac{d}{d\lambda} G_\lambda^A \right) \]
\[ = \frac{d}{d\lambda} \log \det G_\lambda^A.\]
Here we used the fact that \( \frac{d}{d\lambda} (L - \lambda)^{-1} = (L - \lambda)^{-2} \) and \( \det G^\lambda \) is non-zero in \( \lambda \in \mathbb{C} \setminus [\lambda_0, \lambda_\infty] \) by Lemma 2.3.

Next we define a generalized Krein's spectral shift function \( \theta^\lambda (\lambda) \). Recall that for any \( f \in l^2(G, m) \), \( \| (\lambda G + I) f \| \to 0 \) as \( |\lambda| \to \infty \). Then, since \( G^\lambda \) is a finite dimensional matrix, we have

\[
(2.8) \quad \| \lambda G^\lambda + I \| \to 0 \quad \text{as} \quad |\lambda| \to \infty.
\]

Therefore because of the continuity of the determinant, for \( \Im \lambda > 0 \)

\[
(2.9) \quad \det G^\lambda - (-\lambda)^{-|\lambda|} \quad \text{as} \quad |\lambda| \to \infty.
\]

We take the branch of the logarithm so that \( \Im \log \det G^\lambda_{i+\epsilon} \to 0 \) as \( \lambda \to -\infty \).

Let \( \{\nu_k (\lambda)\}_{k=1}^A \) be eigenvalues of \( G^\lambda \). Then, \( \Im \log \det G^\lambda = \sum_{k=1}^A \Im \log \nu_k (\lambda) \).

On the other hand, for each eigenvalue \( \nu_k (\lambda) \), there exists a normalized eigenfunction \( f_k \) such that

\[
(2.4) \quad \nu_k (\lambda) = \langle f_k, G^\lambda f_k \rangle = \int_{\sigma(L)} \frac{1}{\xi - \lambda} \ d\mu_i (\xi).
\]

Here we used (2.4). Then for any \( \Im \lambda > 0 \) and \( 1 \leq k \leq A \), \( \Im \nu_k (\lambda) > 0 \), and since the unordered tuple of eigenvalues is continuous in \( \lambda \), by the way of taking the branch of the logarithm, we have

\[
0 < \Im \log \det G^\lambda < |A| \pi.
\]

Hence, by the Fatou's theorem, a limit

\[
(2.10) \quad \theta^\lambda (\lambda) := \lim_{\epsilon \to 0} \frac{1}{\pi |A|} \Im \log \det G^\lambda_{i+\epsilon}
\]

exists for almost every \( \lambda \in \mathbb{R} \) and \( 0 \leq \theta^\lambda (\lambda) \leq 1 \). We call it a generalized Krein's spectral shift function.

**Lemma 2.7.** For almost every \( \lambda \in \mathbb{R} \), \( \theta^\lambda (\lambda) \) exists and \( 0 \leq \theta^\lambda (\lambda) \leq 1 \). In particular,

\[
\theta^\lambda (\lambda) = \begin{cases} 
0 & \text{if } \lambda < \lambda_0, \\
1 & \text{if } \lambda > \lambda_\infty \end{cases}
\]

*Proof.* We have already shown the existence and so we will show only the second statement. Since \( \det G^\lambda \) is real-valued for \( \lambda \in \mathbb{R} \setminus [\lambda_0, \lambda_\infty] \), by the definition of the \( \theta^\lambda (\lambda) \), we have

\[
(2.11) \quad \theta^\lambda (\lambda) \in \left\{ \frac{k}{|A|}, k \in \mathbb{Z} \right\}.
\]
For any \( x, y \in \mathbb{G} \), the convergence of the green function \( g_{x+i\epsilon}(x, y) \) as \( \epsilon \to 0 \) is uniform on an arbitrary compact set \( K \subset \mathbb{R} \setminus [\lambda_0, \lambda_\omega] \). Then, as \( \epsilon \to 0 \), \( \text{Im} \log \det G_{x+i\epsilon}^A \) also converges uniformly on compact sets in \( \mathbb{R} \setminus [\lambda_0, \lambda_\omega] \). Consequently, \( \theta_\lambda(\lambda) \) is continuous on \( \mathbb{R} \setminus [\lambda_0, \lambda_\omega] \) and in particular, taking account of (2.11), constant on each open intervals \( (-\infty, \lambda_0) \) and \( (\lambda_\omega, \infty) \). Furthermore, by the way of taking the branch of the logarithm and (2.9), we conclude the lemma.

**Theorem 2.8.** Let \( V \) be a real-valued bounded function. Then,

\[
(2.12) \quad \frac{1}{|A|} \sum_{x \in \mathbb{G}} (p^V(t, x, x) - p^\lambda_A(t, x, x)) = e^{-\lambda t} + i \int_{\lambda_0}^{\lambda_\omega} e^{-\lambda t} \theta_\lambda(\lambda) \, d\lambda
\]

where \( \lambda_0 \) (resp. \( \lambda_\omega \)) is the minimum (resp. maximum) of the spectrum of \( L \).

**Proof.** Since \( p^V(t, x, x) \) is the kernel of the operator \( e^{-tL} \), using the Dunford integral, we obtain the following expression:

\[
\sum_{x \in \mathbb{G}} (p^V(t, x, x) - p^\lambda_A(t, x, x)) = -\sum_{x \in \mathbb{G}} \frac{1}{2\pi i} \int_C e^{-\lambda t} (g_\lambda(x, x) - g^A_\lambda(x, x)) \, d\lambda
\]

where the contour \( C \) is

\[
\{\lambda_0 - \delta + i\xi ; -\epsilon \leq \xi \leq \epsilon\} \cup \{\lambda_\omega + \delta + i\xi ; -\epsilon \leq \xi \leq \epsilon\}
\]

\[
\cup \{\xi \pm i\epsilon ; \lambda_0 - \delta \leq \xi \leq \lambda_\omega + \delta\}
\]

for \( \epsilon > 0 \) and \( \delta > 0 \). The interchange of the summation and the integral over \( C \) can be easily justified.

By Proposition 2.6, we have

\[
\sum_{x \in \mathbb{G}} (p^V(t, x, x) - p^\lambda_A(t, x, x)) = -\frac{1}{2\pi i} \int_C e^{-\lambda t} \frac{d}{d\lambda} \log \det G^A_\lambda \, d\lambda.
\]

Now we calculate the right-hand side.

\[
\frac{-1}{2\pi i} \int_C e^{-\lambda t} \frac{d}{d\lambda} \log \det G^A_\lambda \, d\lambda
\]

\[
= \frac{1}{\pi} \int_{\lambda_0 - \delta}^{\lambda_0 + \delta} \text{Im} \left( e^{-(\lambda + i\epsilon)t} \frac{d}{d\lambda} \log \det G^A_{\lambda + i\epsilon} \right) d\lambda
\]

\[
+ \frac{1}{2\pi i} \int_{\lambda_0 - \delta - i\epsilon}^{\lambda_0 - \delta + i\epsilon} e^{-\lambda t} \frac{d}{d\lambda} \log \det G^A_\lambda \, d\lambda
\]

\[
+ \frac{1}{2\pi i} \int_{\lambda_\omega + \delta + i\epsilon}^{\lambda_\omega + \delta - i\epsilon} e^{-\lambda t} \frac{d}{d\lambda} \log \det G^A_\lambda \, d\lambda.
\]
The second and third term of the right-hand side will vanish as $\epsilon \to 0$ since the integrands are analytic in the resolvent set. Integrating the first term by parts, we obtain

$$\frac{1}{\pi} \int_{\lambda_0 - \delta}^{\lambda_0 + \delta} \Im \left( e^{-\epsilon \lambda} \frac{d}{d\lambda} \log \det G^{A+\epsilon}_{\lambda} \right) d\lambda$$

$$= \frac{1}{\pi} \left[ \Im \left( e^{-\epsilon \lambda} \log \det G^{A}_{\lambda} \right) \right]_{\lambda_0 - \delta}^{\lambda_0 + \delta}$$

$$+ \frac{t}{\pi} \int_{\lambda_0 - \delta}^{\lambda_0 + \delta} \Im \left( e^{-\epsilon \lambda} \log \det G^{A}_{\lambda+\epsilon} \right) d\lambda.$$

Note that $\Im \log \det G^{A}_{\lambda}$ is bounded by (2.9). Using the dominated convergence theorem, as $\epsilon \to 0$, we obtain

$$\frac{1}{|A|} \sum_{x \in G} \left( p^V(t, x, x) - p^A_{\lambda}(t, x, x) \right)$$

$$= -e^{-(\lambda_0 - \delta)\Im} \theta_{\lambda} (\lambda_0 - \delta) + e^{-(\lambda_0 + \delta)\Im} \theta_{\lambda} (\lambda_0 + \delta)$$

$$+ \frac{t}{\pi} \int_{\lambda_0 - \delta}^{\lambda_0 + \delta} e^{-\epsilon \lambda} \theta_{\lambda}(\lambda) d\lambda.$$

Hence, from Lemma 2.7, as $\delta \to 0$, the proof is completed.

**Theorem 2.9.** Let $V$ be a real-valued bounded function. Then

$$V(a) = \lambda_\omega - 1 - \int_{\lambda_\omega - \delta}^{\lambda_\omega + \delta} e^{-\epsilon \lambda} \theta_{\lambda}(\lambda) d\lambda.$$  

**Proof.** Differentiating both sides of (2.12) and taking the limit $t \to 0$, we have the result because of Proposition 2.2.

§ 3. An Example

We will give an example which can be calculated $\theta_{\lambda}$ explicitly. This example is essentially due to Craig [2]. Let $G$ be a one-dimensional lattice $\mathbb{Z}^d$ and $A$ be a singleton $\{a\}$. $V$ is a $n$ periodic potential, that is, for fixed $n \geq 1$, $V(x) = V(y)$ if $d(x, y) = n$. In this case it is known that the spectrum of $L$ has a finite band structure. Precisely, the spectrum set is a union of finite closed intervals, for some $N$,

$$\sigma(L) = \bigcup_{0 \leq k \leq N} [\lambda_{2k}, \lambda_{2k+1}].$$
Also, the essential spectrum of $L_a$ is same as that of $L$ and the spectrum of $L_a$ may has eigenvalues. Since the green function $g_2(a, a)$ is taking real value and monotone increasing on each resolvent set $I_k = (\lambda_{2k-1}, \lambda_{2k})$, it has at most one zero on each $I_k$. If there exists a zero on $I_k$, we put it as $\mu_k(a)$ which is an eigenvalue of $L_a$. If $g_2(a, a) > 0$ (resp. $< 0$) on $I_k$, we put $\mu_k(a) = \lambda_{2k}$ (resp. $\lambda_{2k-1}$).

Now we use much weaker version of the remarkable result in [6].

**Theorem 3.1.** Let $V$ be a periodic potential. Then, for a.e. $\lambda \in \sigma(L)$,

$$\lim_{\epsilon \to 0} \text{Re } g_{2+i\epsilon}(a, a) = 0.$$  

For details, one may refer to [6].

Now we can calculate $\theta_a(\lambda)$ as follows:

$$\theta_a(\lambda) = \begin{cases} 
1, & \lambda_{2k-1} < \lambda < \mu_k(a), \\
0, & \mu_k(a) < \lambda < \lambda_{2k}, \\
\frac{1}{2}, & \lambda_{2k} < \lambda < \lambda_{2k+1}.
\end{cases}$$

It follows from Theorem 3.1 and the fact $g_2(a, a)$ is real and monotone increasing on the resolvent set. Then we have the following theorem:

**Corollary 3.2.** Let $G$ be $\mathbb{Z}^1$ and $V$ a periodic potential. Then

$$V(a) = \frac{\lambda_0 + \lambda_w}{2} - 1 + \frac{1}{2} \sum_{1 \leq k \leq N} (\lambda_{2k-1} + \lambda_{2k} - 2\mu_k(a)).$$

**Proof.** By Theorem 2.9 we have

$$V(a) = \frac{\lambda_0 + \lambda_w}{2} - 1 + \int_{\lambda_0}^{\lambda_w} \left( \frac{1}{2} - \theta_a(\lambda) \right) d\lambda.$$  

Noting that $\frac{1}{2} - \theta_a(\lambda)$ vanishes on $\sigma(L)$, we have

$$V(a) = \frac{\lambda_0 + \lambda_w}{2} - 1 + \frac{1}{2} \sum_{k=1}^{N} (\lambda_{2k-1} + \lambda_{2k} - 2\mu_k(a)).$$

**Remark 3.3.** Corollary 3.2 also holds for so-called reflectionless potentials [2].
§ 4. A Discrete Analogue of the Gutzwiller's Trace Formula

Now in order to state a discrete analogue of the Gutzwiller’s trace formula for open system, we define a function $d_4$ on $V(G) \times V(G)$ as follows: for each $\lambda < \inf_{x \in G} V(x)$

$$d_4(x, y) = -\frac{1}{2} \left( \log E_x[e^{-F_i(T_y)}] + \log E_y[e^{-F_i(T_y)}] \right)$$

where $F_i(t) = F_i(t, w) = \int_0^t (-\lambda + V(w)) \, dt$. Remark that since $g_2(x, y) = E_x[e^{-F_i(T_y)} ; T_y < \infty] g_2(y, y)$ and $E_x[e^{-F_i(T_y)} ; T_y < \infty]$ for $\lambda < \inf_{x \in G} V(x)$,

$$d_4(x, y) = -\frac{1}{2} \log \frac{g_2(x, y) g_2(y, x)}{g_2(x, x) g_2(y, y)}.$$ 

Lemma 4.1. Let $\lambda < \inf_{x \in G} V(x)$. Then, $d_4(\cdot, \cdot)$ is a distance, that is, $d_4(\cdot, \cdot) : V(G) \times V(G) \to \mathbb{R}^+$ satisfies the following:

1. $d_4(x, y) \geq 0$ and if $d_4(x, y) = 0$ then $x = y$,
2. $d_4(x, y) = d_4(y, x)$,
3. $d_4(x, y) \leq d_4(x, z) + d_4(z, y)$.

Proof. (1) and (2) are trivial. So we will show the triangle inequality (3).

$$E_x[e^{-F_i(T_y)}] = E_x[e^{-F_i(T_y)} ; T_y < T_x] + E_x[e^{-F_i(T_x)} ; T_y > T_x]$$

$$= E_x[e^{-F_i(T_y)} ; T_y < T_x, T_y < \infty] \cdot E_y[e^{-F_i(T_y)}] + E_x[e^{-F_i(T_x)} ; T_y > T_x].$$

Here we used the strong Markov property.

$$-\log E_x[e^{-F_i(T_y)}]$$

$$= -\log (E_x[e^{-F_i(T_y)} ; T_y < T_x, T_y < \infty] \cdot E_y[e^{-F_i(T_y)}] + E_x[e^{-F_i(T_x)} ; T_y > T_x])$$

$$\leq -\log (E_x[e^{-F_i(T_y)} ; T_y < T_x, T_y < \infty] \cdot E_y[e^{-F_i(T_y)}] + E_x[e^{-F_i(T_y)} ; T_y > T_x]).$$

Note that if $0 < x, a, b \leq 1$ then $-\log (ax + b) \leq -\log (a + b) - \log x$. Then we have

$$-\log E_x[e^{-F_i(T_y)}] \leq -\log E_x[e^{-F_i(T_y)}] - \log E_y[e^{-F_i(T_y)}].$$

Similarly, we have

$$-\log E_x[e^{-F_i(T_y)}] \leq -\log E_x[e^{-F_i(T_y)}] - \log E_y[e^{-F_i(T_y)}].$$

Then, we obtain the lemma.

It is easy to see that
We are interested in the detailed asymptotic properties of the family of distances \( \{d_i\} \). However, we just give an easy example of \( \{d_i\} \) which can be explicitly calculated.

**Example 4.2.** Let \( G \) be a \( d \)-regular tree and \( V \) is identically zero. Let \( \alpha_d = \frac{2\sqrt{d-1}}{d} \). Then as is well known, the spectrum of \(-\Delta_d\) is \([1-\alpha_d, 1+\alpha_d]\).

By an easy calculation we obtain

\[
d_{\lambda}(x,y) = d(x,y) \cdot (-\log m_d(\lambda))
\]

for \( \lambda < 0 \). Here \( d(x,y) \) is the same one defined by (2.2) and

\[
m_d(\lambda) = \frac{d}{2d-2} \left( 1 - \frac{\lambda}{\sqrt{1-\lambda^2-\alpha_d^2}} \right).
\]

Especially, as \( \lambda \to 0 \)

\[
\lim_{\lambda \to 0} d_{\lambda}(x,y) = d(x,y) \cdot \log(d-1) \quad \text{if } d \geq 3,
\]

\[
\lim_{\lambda \to 0} d_{\lambda}(x,y) = d(x,y) \quad \text{if } d = 2
\]

and as \( \lambda \to -\infty \)

\[
d_{\lambda}(x,y) \sim d(x,y) \left\{ \log(1-\lambda) + \log d - \frac{1}{4} \left( \frac{\alpha_d}{1-\lambda} \right)^2 - \cdots \right\}.
\]

Now let us show a discrete version of the Gutzwiller's trace formula for our setting. Let \( G_d^\lambda \) be the matrix that was defined in Lemma 2.3. We decompose \( G_d^\lambda \) into two matrices \( D_d^\lambda \) and \( K_d^\lambda \) as follows:

\[
G_d^\lambda = D_d^\lambda (I + K_d^\lambda)
\]

where \( D_d^\lambda \) is the diagonal matrix such that \( (D_d^\lambda)_{a,a} = g_d(a,a) \) for \( a \in \Lambda \) and

\[
(K_d^\lambda)_{a,b} = \begin{cases} \frac{g_d(a,b)}{g_d(b,b)} & \text{if } a \neq b, \\ 0 & \text{if } a = b. \end{cases}
\]

Then,

**Lemma 4.3.** There exists \( \tilde{\lambda} \in \mathbb{R} \) such that for any \( \lambda < \tilde{\lambda} \)

\[
\| K_d^\lambda \| < 1.
\]
Proof. It is obvious by (2.9).

Before we state our theorem, we prepare some notations. Let \( \sigma \) be the shift transformation on \( A^N = \{ a = (a_n)_{n \in \mathbb{N}} : a_n \in A \} \), i.e.,
\[
(\sigma a)_n = a_{n+1} \quad (n \in \mathbb{N}).
\]
Let \( \Sigma \) be the \( \sigma \)-invariant closed subset of \( A^N \) such that
\[
\Sigma = \{ a \in A^N : a_n \neq a_{n+1} \text{ for any } n \in \mathbb{N} \}.
\]
The restriction of \( \sigma \) on \( \Sigma \) will be denoted again by \( \sigma \). For a pair \( (\Sigma, \sigma) \) we define
\[
F(n) = \{ a \in \Sigma : \sigma^n a = a \}
\]
\[
P(n) = F(n) \cup \bigcup_{k | n} F(k)
\]
where \( k | n \) means that \( k \) is a divisor of \( n \). For \( a, b \in P(n) \) we define the equivalence relation by
\[
a \sim b \iff \exists 0 \leq k \leq n - 1 \text{ such that } \sigma^k a = b.
\]
Let \( \Gamma_n = P(n) / \sim \) be the equivalence class of \( P(n) \) by \( \sim \). We call an element \( \gamma \) of \( \Gamma_n \) a prime periodic orbits with period \( n \) and denote the period of \( \gamma \) by \( L_\gamma \). The totality of prime periodic orbits is denoted by \( \Gamma \). Then, our theorem is the following:

**Theorem 4.4.** There exists \( \bar{\lambda} \in \mathbb{R} \) such that for any \( \lambda < \bar{\lambda} \)
\[
\sum_{x \in \mathcal{O}} (g_2(x, x) - g_2(x, x)) = \sum_{a \in A} \frac{d}{d\lambda} \log g_2(a, a)
\]
\[
+ \sum_{r \in \Gamma} \frac{dS_r(\lambda)}{d\lambda} \sum_{n \geq 1} \exp(-nS_r(\lambda) - n\pi i L_\gamma)
\]
where \( S_r(\lambda) \) is the length of a periodic orbit \( \gamma \) with respect to the distance \( d_r \).

Proof. Since \( \|K_\lambda^2\| < 1 \) for \( \lambda < \bar{\lambda} \), we have
\[
\det(I + K_\lambda^2) = \det \exp \log(I + K_\lambda^2) = \exp(\text{Tr} \log(I + K_\lambda^2)).
\]
\[
= \exp \left( - \sum_{n=1}^{\infty} \frac{(-1)^n}{n} \text{Tr} (K_\lambda^n) \right).
\]
By the definition of \( K_\lambda^2 \), we obtain
\[
\text{Tr} (K_\lambda^n) = \sum_{\gamma \in \Gamma_n} \prod_{i=1}^n E_n[e^{-F_i/T_\gamma(i)}]
\]
where $a_1 a_2 \ldots a_N$ is a periodic point and $a_{N+1} = a_1$. Noting that $S_{\gamma^*}(\lambda) = S_{\gamma}(\lambda) + S_{\gamma}(\lambda)$ we obtain

$$\det(I + K^2_\lambda) = \exp\left( -\sum_{n=1}^{\infty} \frac{1}{n} \sum_{\tau \in \Gamma(n)} e^{-\langle S_{\tau}(\lambda^1 + \pi L)\rangle} \right)$$

$$= \exp\left( -\sum_{n=1}^{\infty} \frac{1}{n} \sum_{\tau \in \Gamma(n)} e^{-\langle S_{\tau}(\lambda^1 + \pi L)\rangle} \right)$$

$$= \exp\left( -\sum_{k=1}^{\infty} \sum_{\tau \in \Gamma} \sum_{m=1}^{\infty} \frac{1}{m} e^{-\langle S_{\tau}(\lambda^1 + \pi L)\rangle} \right)$$

$$= \prod_{\tau \in \Gamma} \left( 1 - e^{-\langle S_{\tau}(\lambda^1 + \pi L)\rangle} \right).$$

Hence taking the logarithm and differentiating both sides of the equation above, we complete our proof.

**Remark 4.5.** For fixed $\lambda < \lambda$ the Fredholm determinant $\det(I - zK^2_\lambda)$ is the reciprocal of the Ruelle zeta function for the potential $U(a) = \langle a_1, a_2 \rangle + i\pi$. Here the Ruelle zeta function $\zeta(z)$ is defined by

$$\zeta(z) = \exp\left( -\sum_{n=1}^{\infty} \frac{z^n}{n} \sum_{\tau \in \Gamma(n)} e^{-\langle S_{\tau}(U)\rangle} \right)$$

where $S_n U(a) = \sum_{k=0}^{n-1} U(\sigma^k a)$ [1].

**References**


