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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 $L^2(\mathbf{R}^1)$ and L_a that is imposed the Dirichlet condition at $a\in\mathbf{R}^1$ has a relation

$$(1.1)\qquad \mathrm{Tr}(L-L_a)=V(a)=\lambda_0+\sum_{j=1}^{\infty}(\lambda_{2j}+\lambda_{2j-1}-2\mu_j)$$

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 Δ_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*

$$(1.2)\qquad \frac{1}{|A|}\mathrm{Tr}(L-L_A)=\frac{1}{|A|}\sum_{a\in A}V(a)=\lambda_\infty-1-\int_{\lambda_0}^{\lambda_\infty}\theta_A(\lambda)\,d\lambda$$

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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 $\mathrm{Tr}(G_\lambda - G_\lambda^A)$ can be expanded by the periodic orbits on A where G_λ (resp. G_λ^A) is the resolvent of the operator L (resp. L_A).

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

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

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

where Γ is the set of all prime periodic orbits, L_γ is the period of γ and $S_\gamma(\lambda)$ is the length of a periodic orbit γ with respect to the distance d_λ 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 $\{m(x)\}_{x\in G}$ 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

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

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

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

Let V be a real-valued bounded function and we define a discrete Schrödinger operator by

$$L=-\Delta_G+V.$$

It is a linear bounded self-adjoint operator on $l^2(G, m)$.

Let $A\subset G$ be a finite subset of G. We consider two problems for our operator, i.e., one is

$$L\phi(x)=\lambda\phi(x) \qquad x\in G$$

and the other is

$$\begin{cases} L_A\phi(x)=L\phi(x)=\lambda\phi(x) & x\in G\backslash A \\ L_A\phi(a)=0 \quad a\in A, \end{cases}$$

and their domains are $D(L)=l^2(G, m)$ and $D(L_A)=\{f\in l^2(G, m); f(a)=0$ for any $a\in A\}$. We denote the fundamental solutions of the associated heat equations by $p^V(t, x, y)$ and $p_A^V(t, x, y)$, respectively, and the associated green functions, that is, the integral kernels of $(L-\lambda)^{-1}$ and $(L_A-\lambda)^{-1}$ by $g_\lambda(x, y)$ and $g_\lambda^A(x, y)$, 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

$$\sup_{x\in G}|\{r\in G; p(x, r)>0\}|\leq M \tag{2.1}$$

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 $\sum_{x\in G}(p^V(t, x, x)-p_A^V(t, x, x))$ 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 Δ_G, and T_A the first hitting time to the set A. Then, as $t\to 0$,*

$$E_a[\delta_a(w_t)]=1-t+O(t^2)$$

and

$$\sum_{x\in G\backslash A}E_x[\delta_x(w_t); T_A\leq t]=O(t^2)$$

where $\delta_x(\cdot)$ is the indicator function of $x\in G$.

Proof. Firstly, since Δ_G is the generator of w_t and is bounded, we have

$$\begin{aligned} E_a[\delta_a(w_t)] &= \sum_{n\geq 0}\frac{t^n}{n!}\Delta_G{}^n\delta_a(a) \\ &=1+t\ (\Delta_G\delta_a)(a)+O(t^2) \\ &=1-t+O(t^2) \end{aligned}$$

as $t\to 0$.

Secondly, we define a metric on G as follows: for any $x, y\in G$

$$(2.2) \qquad d(x, y) = \inf\left\{ \begin{matrix} n \geq 0; & \exists \text{ path } x = x_0\, x_1 \dots x_n = y \\ & \text{s.t. } p(x_i, x_{i+1}) > 0 \quad 0 \leq \forall i \leq n-1 \end{matrix} \right\}.$$

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

$$\sum_{x \in G \setminus A} E_x[\delta_x(w_t); T_A \leq t] = \sum_{n \geq 1} \sum_{\substack{x \in G \\ d(x,A)=n}} E_x[\delta_x(w_t); T_A \leq t]$$

$$\leq \sum_{n \geq 1} |A| M^n P_x[w \text{ has at least } 2n \text{ jumps up to time } t]$$

$$= \sum_{n \geq 1} |A| M^n \sum_{k \geq 2n} \frac{e^{-t} t^k}{k!} \leq \sum_{n \geq 1} |A| M^n t^{2n} \leq Ct^2 \quad \text{as } t \to 0.$$

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,*

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

where $|A|$ is the cardinality of the set A.

Proof. By the Feynman-Kac formula, we have

$$p^V(t, x, x) - p_A^V(t, x, x) = E_x[e^{-\int_0^t V(w_s) ds}(1 - \chi_{\{T_A > t\}}) \delta_x(w_t)]$$

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

$$\begin{aligned} &\sum_{x \in G} (p^V(t, x, x) - p_A^V(t, x, x)) \\ &= \sum_{x \in G} E_x[e^{-\int_0^t V(w_s) ds} (1 - \chi_{\{T_A > t\}}) \delta_x(w_t)] \\ &= \sum_{x \in G} \sum_{n \geq 0} \frac{(-1)^n}{n!} E_x\left[\left(\int_0^t V(w_s) ds\right)^n (1 - \chi_{\{T_A > t\}}) \delta_x(w_t)\right]. \end{aligned}$$

For $n = 0$, by using Lemma 2.1 we have

$$\begin{aligned} &\sum_{x \in G} E_x[(1 - \chi_{\{T_A > t\}}) \delta_x(w_t)] \\ &= \sum_{a \in A} E_a[\delta_a(w_t)] + \sum_{x \in G \setminus A} E_x[\delta_x(w_t); T_A \leq t] \\ &= |A|(1 - t) + O(t^2) \qquad \text{as } t \to 0. \end{aligned}$$

For $n = 1$, we have

$$\sum_{x\in G} E_x\Big[\Big(\int_0^t V(w_s)\,ds\Big)(1-\chi_{\{T_A>t\}})\,\delta_x(w_t)\Big]$$

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

$$-p^0_A(s,x,y)V(y)p^0_A(t-s,y,x))$$

where $p^0(t, x, y)$ and $p^0_A(t, x, y)$ are the heat kernels for the case that the potential V is identically zero. Using the semigroup property, we have

$$=\int_0^t ds \sum_{y\in G} V(y)\,(p^0(t,y,y)-p^0_A(t,y,y))$$

$$=t\Big\{\sum_{a\in A} V(a)E_a[\delta_a(w_t)]+\sum_{y\in G\setminus A} V(x)E_x[\delta_x(w_t);\, T_A\le t]\Big\}$$

$$=t\sum_{a\in A}V(a)+O(t^2)\quad \text{as } t\longrightarrow 0.$$

Last we estimate the term for $n\ge 2$.

$$\Big|\sum_{n\ge 2}\frac{(-1)^n}{n!}\sum_{x\in G}E_x\Big[\Big(\int_0^t V(w_s)\,ds\Big)^n(1-\chi_{\{T_A>t\}})\,\delta_x(w_t)\Big]\Big|$$

$$\le \sum_{n\ge 2}\frac{t^n}{n!}\|V\|^n_\infty \sum_{x\in G}E_x[(1-\chi_{\{T_A>t\}})\,\delta_x(w_t)]$$

$$\le Ct^2.$$

Then, we have

$$\sum_{x\in G}(p^V(t,x,x)-p^V_A(t,x,x))=|A|-t(\sum_{a\in A}V(a)+|A|)+O(t^2)\quad \text{as } t\longrightarrow 0.$$

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

Proof. Note that $g_\lambda(x,y)$ is holomorphic in $\lambda\in\mathbf{C}\setminus\sigma(L)$. It is obvious by the definition of the determinant that $\det G^A_\lambda$ is also holomorphic in $\lambda\in\mathbf{C}\setminus\sigma(L)$. Recall that

$$g_\lambda(x,y)=\left(\frac{m(y)}{m(x)}\right)^{1/2}\int_{\sigma(L)}\frac{1}{\xi-\lambda}d\langle E(\xi)e_x,e_y\rangle \tag{2.3}$$

where $\{e_x\}_{x\in G}$ is an orthonormal basis of $l^2(G,m)$ 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 $l^2(A,m)$. Let $f\in l^2(G,m)$ be the extension of f_0 such that $supp\, f\subset A$, $f(a)=f_0(a)$ for any $a\in A$ and $\|f\|=1$. Then we have

$$\langle f_0, G_\lambda^A f_0\rangle_A=\langle f, G_\lambda f\rangle=\int_{\sigma(L)}\frac{1}{\xi-\lambda}d\mu_f(\xi) \tag{2.4}$$

where $d\mu_f(\xi)=d\|E(\xi)f\|^2$. We will estimate $|\langle f, G_\lambda f\rangle|$ from below. Firstly, in the case that $|\mathrm{Im}\lambda|>0$, for any $f\in l^2(G,m)$, we have

$$|\langle f, G_\lambda f\rangle| \geq \left|\int_{\sigma(L)}\frac{\mathrm{Im}\lambda}{|\xi-\lambda|^2}d\mu_f(\xi)\right|$$

$$\geq \frac{|\mathrm{Im}\lambda|}{\max_{\xi\in\sigma(L)}|\xi-\lambda|^2}. \tag{2.5}$$

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 λ such that $|\langle G_\lambda f, f\rangle|\geq C(\lambda)>0$. Then, for any $\lambda\in\mathbb{C}\setminus[\lambda_0,\lambda_\infty]$, $\det G_\lambda^A\neq 0$.

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

Lemma 2.5. $\lambda\in\mathbb{C}\setminus[\lambda_0,\lambda_\infty]$. *Then for any* $x,y\in G$

$$g_\lambda(x,y)-g_\lambda^A(x,y)=\sum_{a\in A} g_\lambda(x,a)\,(G_\lambda^A)^{-1}\,g_\lambda(a,y) \tag{2.6}$$

where $(G_\lambda^A)^{-1}$ *acts on the first variable.*

Proof. Let $F_\lambda(t)=F_\lambda(t,w)=\int_0^t(-\lambda+V(w_t))dt$. If $\lambda<\inf_{x\in G}V(x)$, $F_\lambda(t)>0$, and so $F_\lambda(\infty)=\infty$. For any $\lambda<\inf_{x\in G}V(x)$, by the strong Markov property, we have

$$g_\lambda(x,y)-g_\lambda^A(x,y)=E_x\left[\int_{T_A}^\infty e^{-F_\lambda(t)}\delta_y(w_t)\,dt\right]$$

$$=E_x\left[e^{-F_\lambda(T_A)}E_x\left[\int_0^\infty e^{-F_\lambda(t,S_{T_A}w_t)}\delta_y(S_{T_A}w_t)\,dt \mid \mathscr{F}_{T_A}\right];\ T_A<\infty\right]$$

$$=E_x\left[e^{-F_\lambda(T_A)}E_{w_{T_A}}\left[\int_0^\infty e^{-F_\lambda(t)}\delta_y(w_t)\,dt\right];\ T_A<\infty\right]=E_x\left[e^{-F_\lambda(T_A)}g_\lambda(w_{T_A},y);\ T_A<\infty\right]$$

where $(S_s w)_t=w_{t+s}$. We put $\mu_{x,\lambda}(a)=E_x[e^{-F_\lambda(T_A)};\ w_{T_A}=a,\ T_A<\infty]$ 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_λ^A. Then we have

$$\begin{aligned}
&\sum_{a\in A}g_\lambda(x,a)\,(G_\lambda^A)^{-1}g_\lambda(a,y)\\
&=\sum_{a\in A}\sum_{b\in A}g_\lambda(b,a)\mu_{x,\lambda}(b)\,(G_\lambda^A)^{-1}\,g_\lambda(a,y)\\
&=\sum_{b\in A}\mu_{x,\lambda}(b)\sum_{a\in A}g_\lambda(b,a)\,(G_\lambda^A)^{-1}g_\lambda(a,y)\\
&=\sum_{b\in A}\mu_{x,\lambda}(b)g_\lambda(b,y)=g_\lambda(x,y)-g_\lambda^A(x,y).
\end{aligned}$$

The lemma is obtained by analytic continuation.

Proposition 2.6. *Let* $\lambda\in\mathbf{C}\setminus[\lambda_0,\lambda_\infty]$. *Then*

$$\sum_{x\in G}(g_\lambda(x,x)-g_\lambda^A(x,x))=\frac{d}{d\lambda}\log\det G_\lambda^A. \tag{2.7}$$

Proof. Since $(G_\lambda^A)^{-1}$ is a linear operator, taking summation over $x\in G$, we have

$$\begin{aligned}
\sum_{x\in G}(g_\lambda(x,x)-g_\lambda^A(x,x))&=\sum_{x\in G}\sum_{a\in A}g_\lambda(x,a)\,(G_\lambda^A)^{-1}g_\lambda(a,x)\\
&=\sum_{a\in A}(G_\lambda^A)^{-1}\frac{d}{d\lambda}G_\lambda^A(a,a)=\mathrm{Tr}\left((G_\lambda^A)^{-1}\frac{d}{d\lambda}G_\lambda^A\right)\\
&=\frac{d}{d\lambda}\log\det G_\lambda^A.
\end{aligned}$$

Here we used the fact that $\frac{d}{d\lambda}(L-\lambda)^{-1}=(L-\lambda)^{-2}$ and $\det G_\lambda^A$ 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 $\theta_A(\lambda)$. Recall that for any $f \in l^2(G, m)$, $\|(\lambda G_\lambda + I)f\| \to 0$ as $|\lambda| \to \infty$. Then, since G_λ^A is a finite dimensional matrix, we have

$$\|\lambda G_\lambda^A + I\| \to 0 \text{ as } |\lambda| \to \infty. \tag{2.8}$$

Therefore because of the continuity of the determinant, for $\mathrm{Im}\lambda > 0$

$$\det G_\lambda^A \sim (-\lambda)^{-|A|} \text{ as } |\lambda| \to \infty. \tag{2.9}$$

We take the branch of the logarithm so that $\mathrm{Im} \log\det G_{\lambda+\iota\epsilon}^A \to 0$ as $\lambda \to -\infty$. Let $\{\nu_k(\lambda)\}_{k=1}^{|A|}$ be eigenvalues of G_λ^A. Then, $\mathrm{Im}\ \log\det G_\lambda^A = \sum_{k=1}^{|A|} \mathrm{Im}\ \log\ \nu_k(\lambda)$. On the other hand, for each eigenvalue $\nu_k(\lambda)$, there exists a normalized eigenfunction f_k such that

$$\nu_k(\lambda) = \langle f_k, G_\lambda^A f_k \rangle_A = \int_{\sigma(L)} \frac{1}{\xi - \lambda} d\mu_{f_k}(\xi).$$

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

$$0 < \mathrm{Im}\ \log\ \det\ G_\lambda^A < |A|\pi.$$

Hence, by the Fatou's theorem, a limit

$$\theta_A(\lambda) := \lim_{\epsilon\to 0} \frac{1}{\pi|A|} \mathrm{Im}\ \log\ \det\ G_{\lambda+\iota\epsilon}^A \tag{2.10}$$

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

Lemma 2.7. *For almost every $\lambda \in \mathbb{R}$, $\theta_A(\lambda)$ exists and $0 \le \theta_A(\lambda) \le 1$. In particular,*

$$\theta_A(\lambda) = \begin{cases} 0 & \text{if } \lambda < \lambda_0, \\ 1 & \text{if } \lambda > \lambda_\infty. \end{cases}$$

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

$$\theta_A(\lambda) \in \left\{ \frac{k}{|A|}; k \in \mathbb{Z} \right\}. \tag{2.11}$$

For any $x, y \in G$, the convergence of the green function $g_{\lambda+i\epsilon}(x, y)$ as $\epsilon \to 0$ is uniform on an arbitrary compact set $K \subset \mathbf{R} \setminus [\lambda_0, \lambda_\infty]$. Then, as $\epsilon \to 0$, Im log det $G^A_{\lambda+i\epsilon}$ also converges uniformly on compact sets in $\mathbf{R} \setminus [\lambda_0, \lambda_\infty]$. Consequently, $\theta_A(\lambda)$ is continuous on $\mathbf{R} \setminus [\lambda_0, \lambda_\infty]$ and in particular, taking account of (2.11), constant on each open intervals $(-\infty, \lambda_0)$ and (λ_∞, ∞). 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,*

$$\frac{1}{|A|} \sum_{x \in G} (p^V(t, x, x) - p^V_A(t, x, x)) = e^{-\lambda_\infty t} + t \int_{\lambda_0}^{\lambda_\infty} e^{-\lambda t} \theta_A(\lambda) d\lambda \tag{2.12}$$

where λ_0 (resp. λ_∞) 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:

$$\sum_{x \in G} (p^V(t, x, x) - p^V_A(t, x, x))$$

$$= -\sum_{x \in G} \frac{1}{2\pi i} \int_C e^{-\lambda t} (g_\lambda(x, x) - g^A_\lambda(x, x)) d\lambda$$

where the contour C is

$$\{\lambda_0 - \delta + i\xi ; -\epsilon \leq \xi \leq \epsilon\} \cup \{\lambda_\infty + \delta + i\xi ; -\epsilon \leq \xi \leq \epsilon\}$$

$$\cup \{\xi \pm i\epsilon ; \lambda_0 - \delta \leq \xi \leq \lambda_\infty + \delta\}$$

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

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

Now we calculate the right-hand side.

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

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

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

$$+ \frac{1}{2\pi i} \int_{\lambda_\infty + \delta + i\epsilon}^{\lambda_\infty + \delta - i\epsilon} e^{-\lambda t} \frac{d}{d\lambda} \log \det G^A_\lambda \, d\lambda.$$

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

$$\frac{1}{\pi}\int_{\lambda_0-\delta}^{\lambda_\infty+\delta}\mathrm{Im}\left(e^{-(\lambda+i\epsilon)t}\frac{d}{d\lambda}\log\det G^A_{\lambda+i\epsilon}\right)d\lambda$$

$$=\frac{1}{\pi}\left[\mathrm{Im}\left(e^{-(\lambda+i\epsilon)t}\log\det G^A_{\lambda+i\epsilon}\right)\right]_{\lambda_0-\delta}^{\lambda_\infty+\delta}$$

$$+\frac{t}{\pi}\int_{\lambda_0-\delta}^{\lambda_\infty+\delta}\mathrm{Im}\left(e^{-(\lambda+i\epsilon)t}\log\det G^A_{\lambda+i\epsilon}\right)d\lambda.$$

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

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

$$=-e^{-(\lambda_0-\delta)t}\theta_A(\lambda_0-\delta)+e^{-(\lambda_\infty+\delta)t}\theta_A(\lambda_\infty+\delta)$$

$$+t\int_{\lambda_0-\delta}^{\lambda_\infty+\delta}e^{-\lambda t}\theta_A(\lambda)\,d\lambda.$$

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*

$$\frac{1}{|A|}\sum_{a\in A}V(a)=\lambda_\infty-1-\int_{\lambda_0}^{\lambda_\infty}\theta_A(\lambda)\,d\lambda. \tag{2.13}$$

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 θ_A (λ) explicitly. This example is essentially due to Craig [2]. Let G be a one-dimensional lattice $\mathbb{Z}^1$ 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 $g_\lambda(a, a)$ 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 $g_\lambda(a, a) > 0$ (resp. <0) on I_k, we put $\mu_k(a) = \lambda_{2k}$ (resp. λ_{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. $\lambda \in \sigma(L)$,*

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

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 $g_\lambda(a, a)$ is real and monotone increasing on the resolvent set. Then we have the following theorem:

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

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

Proof. By Theorem 2. 9 we have

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

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

$$V(a) = \frac{\lambda_0 + \lambda_\infty}{2} - 1 + \sum_{k=1}^{N} \int_{\lambda_{2k-1}}^{\lambda_{2k}} \left(\frac{1}{2} - \theta_A(\lambda)\right) d\lambda$$

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

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_λ on $V(G) \times V(G)$ as follows: for each $\lambda < \inf_{x\in G} V(x)$

$$(4.1) \qquad d_\lambda(x, y) = -\frac{1}{2}\Big(\log E_x[e^{-F_\lambda(T_y)}] + \log E_y[e^{-F_\lambda(T_x)}]\Big)$$

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

$$d_\lambda(x, y) = -\frac{1}{2}\log\frac{g_\lambda(x, y)g_\lambda(y, x)}{g_\lambda(x, x)g_\lambda(y, y)}.$$

Lemma 4.1. *Let $\lambda < \inf_{x\in G} V(x)$. Then, $d_\lambda(\cdot, \cdot)$ is a distance, that is, $d_\lambda(\cdot, \cdot) : V(G) \times V(G) \to \mathbb{R}^+$ satisfies the following:*
(1) $d_\lambda(x, y) \geq 0$ and if $d_\lambda(x, y) = 0$ then $x = y$,
(2) $d_\lambda(x, y) = d_\lambda(y, x)$,
(3) $d_\lambda(x, y) \leq d_\lambda(x, z) + d_\lambda(z, y)$.

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

$$\begin{aligned} E_x[e^{-F_\lambda(T_z)}] &= E_x[e^{-F_\lambda(T_z)}; T_y < T_z] + E_x[e^{-F_\lambda(T_z)}; T_y > T_z] \\ &= E_x[e^{-F_\lambda(T_y)}; T_y < T_z, T_y < \infty] \cdot E_y[e^{-F_\lambda(T_z)}] + E_x[e^{-F_\lambda(T_z)}; T_y > T_z]. \end{aligned}$$

Here we used the strong Markov property.

$$\begin{aligned} &-\log E_x[e^{-F_\lambda(T_z)}] \\ &\quad = -\log\,(E_x[e^{-F_\lambda(T_y)}; T_y < T_z, T_y < \infty] \cdot E_y[e^{-F_\lambda(T_z)}] + E_x[e^{-F_\lambda(T_z)}; T_y > T_z]) \\ &\quad \leq -\log\,(E_x[e^{-F_\lambda(T_y)}; T_y < T_z, T_y < \infty] \cdot E_y[e^{-F_\lambda(T_z)}] + E_x[e^{-F_\lambda(T_y)}; T_y > T_z]). \end{aligned}$$

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

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

Similarly, we have

$$-\log E_z[e^{-F_\lambda(T_x)}] \leq -\log E_z[e^{-F_\lambda(T_y)}] - \log E_y[e^{-F_\lambda(T_x)}].$$

Then, we obtain the lemma.

It is easy to see that

$$d_{\lambda_1} > d_{\lambda_2} \quad \text{if } \lambda_1 < \lambda_2 < \inf_{x \in G} V(x). \tag{4.2}$$

We are interested in the detailed asymptotic properties of the family of distances $\{d_\lambda\}$. However, we just give an easy example of $\{d_\lambda\}$ 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 $-\Delta_G$ is $[1-\alpha_d, 1+\alpha_d]$. By an easy calculation we obtain

$$d_\lambda(x, y) = d(x, y) \cdot (-\log m_d(\lambda)) \tag{4.3}$$

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

$$m_d(\lambda) = \frac{d}{2d-2}\left(1-\lambda-\sqrt{(1-\lambda)^2-\alpha_d^2}\right). \tag{4.4}$$

Especially, as $\lambda \to 0$

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

(2) $\lim_{\lambda\to 0-} \frac{d_\lambda(x, y)}{\sqrt{-2\lambda}} = d(x, y) \quad \text{if } d = 2$

and as $\lambda \to -\infty$

$$d_\lambda(x, y) \sim d(x, y)\left\{\log(1-\lambda) + \log d - \frac{1}{4}\left(\frac{\alpha_d}{1-\lambda}\right)^2 - \cdots\right\}. \tag{4.5}$$

Now let us show a discrete version of the Gutzwiller's trace formula for our setting. Let G_λ^A be the matrix that was defined in Lemma 2.3. We decompose G_λ^A into two matrices D_λ^A and K_λ^A as follows:

$$G_\lambda^A = D_\lambda^A\ (I + K_\lambda^A)$$

where D_λ^A is the diagonal matrix such that $(D_\lambda^A)_{a,a} = g_\lambda(a, a)$ for $a \in A$ and

$$(K_\lambda^A)_{a,b} = \begin{cases} \dfrac{g_\lambda(a, b)}{g_\lambda(b, b)} & \text{if } a \neq b, \\ 0 & \text{if } a = b. \end{cases}$$

Then,

Lemma 4.3. *There exists $\tilde{\lambda} \in \mathbf{R}$ such that for any $\lambda < \tilde{\lambda}$*

$$\|K_\lambda^A\| < 1.$$

Proof. It is obvious by (2. 9).

Before we state our theorem, we prepare some notations. Let σ be the shift transformation on $A^{\mathrm{N}}=\{\underline{a}=(a_n)_{n\in\mathrm{N}};\ a_n\in A\}$, i.e.,

$$(\sigma\underline{a})_n=a_{n+1} \quad (n\in\mathbb{N}).$$

Let Σ be the σ-invariant closed subset of A^{N} such that

$$\Sigma=\{\underline{a}\in A^{\mathrm{N}}\ ;\ a_n\neq a_{n+1} \text{ for any } n\in\mathbb{N}\}.$$

The restriction of σ on Σ will be denoted again by σ. For a pair (Σ,σ) we define

$$F(n)=\{\underline{a}\in\Sigma\ ;\ \sigma^n\underline{a}=\underline{a}\}$$

$$P(n)=F(n)\setminus\bigcup_{k|n}F(k)$$

where $k|n$ means that k is a divisor of n. For $\underline{a}, \underline{b}\in P(n)$ we define the equivalence relation by

$$\underline{a}\sim\underline{b}\Leftrightarrow 0\leq\exists k\leq n-1 \text{ such that } \sigma^k\underline{a}=\underline{b}.$$

Let $\Gamma_n=P(n)/\sim$ be the equivalence class of $P(n)$ by $\sim$. We call an element γ of Γ_n a prime periodic orbits with period n and denote the period of γ by L_γ. The totality of prime periodic orbits is denoted by Γ. Then, our theorem is the following:

Theorem 4.4. *There exists $\tilde{\lambda}\in\mathbb{R}$ such that for any $\lambda<\tilde{\lambda}$*

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

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

where $S_\gamma(\lambda)$ is the length of a periodic orbit γ with respect to the distance d_λ.

Proof. Since $\|K_\lambda^A\|<1$ for $\lambda<\tilde{\lambda}$, we have

$$\det(I+K_\lambda^A)=\det\exp\log(I+K_\lambda^A)=\exp(\mathrm{Tr}\log(I+K_\lambda^A)).$$

$$=\exp\left(-\sum_{n=1}^{\infty}\frac{(-1)^n}{n}\mathrm{Tr}(K_\lambda^{A^n})\right).$$

By the definition of K_λ^A, we obtain

$$\mathrm{Tr}(K_\lambda^{A^n})=\sum_{a_1a_2\ a_n\in F(n)}\prod_{i=1}^{n}E_{a_i}[e^{-F_\lambda(T_{a_{i+1}})}]$$

where $\dot{a}_1 a_2 \dots \dot{a}_n$ is a periodic point and $a_{n+1}=a_1$. Noting that $S_{\gamma_1\gamma_2}(\lambda)=S_{\gamma_1}(\lambda)+S_{\gamma_2}(\lambda)$ we obtain

$$\det(I+K_\lambda^A) = \exp\left(-\sum_{n=1}^{\infty}\frac{1}{n}\sum_{\gamma\in F(n)} e^{-(S_\gamma(\lambda)+i\pi L_\gamma)}\right)$$

$$= \exp\left(-\sum_{n=1}^{\infty}\frac{1}{n}\sum_{\substack{\gamma\in P(k)\\ k|n}} e^{-\frac{n}{k}(S_\gamma(\lambda)+i\pi L_\gamma)}\right)$$

$$= \exp\left(-\sum_{k=1}^{\infty}\sum_{\gamma\in\Gamma_k}\sum_{m=1}^{\infty}\frac{1}{m}e^{-m(S_\gamma(\lambda)+i\pi L_\gamma)}\right)$$

$$= \prod_{\gamma\in\Gamma}\left(1-e^{-(S_\gamma(\lambda)+i\pi L_\gamma)}\right).$$

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

Remark 4.5. For fixed $\lambda<\tilde{\lambda}$ the Fredholm determinant $\det(I-zK_\lambda^A)$ is the reciprocal of the Ruelle zeta function for the potential $U(\underline{a})=d_\lambda(a_1, a_2)+i\pi$. Here the Ruelle zeta function $\zeta(z)$ is defined by

$$\zeta(z)=\exp\left(-\sum_{n=1}^{\infty}\frac{z^n}{n}\sum_{\underline{a}\in F(n)} e^{-S_nU(\underline{a})}\right)$$

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

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