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Tunneling on graphs: an approach “à la Helffer-Sjöstrand”

Yves Colin de Verdière *

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Introduction

In the paper [2], the authors study the tunneling effect on a finite graph G . In order to evaluate the eigenvalues of a Schrödinger operator on G in the semi-classical regime, they introduce a kind of Dirichlet to Neumann map which gives an implicit equation. On the other hand, Bernard Helffer and Johannes Sjöstrand gave a very explicit approach to the estimation of the eigenvalues of a semi-classical Schrödinger operator in \mathbb{R}^d in several papers. In particular, in [3], they introduce the so-called interaction matrix whose eigenvalues are close to the tunneling eigenvalues.

The goal of this note is to show that the Helffer-Sjöstrand approach is also suitable for the problem on graphs and to describe how to compute explicitly the interaction matrix.

1 The problem

We consider a finite non-oriented graph $G = (X, E)$ with no loops and we denote by $d(x)$ the degree of the vertex x and by $D(x, y)$ the combinatorial distance between the vertices x and y . A Schrödinger operator H on G is defined by

$$H = \hbar^2 \Delta + V ,$$

where

- \hbar is a positive parameter. The *semi-classical limit* that we will study is $\hbar \rightarrow 0$.

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- Δ is the linear symmetric operator on \mathbb{R}^X defined by

$$\Delta f(x) = - \sum_{y \sim x} f(y) .$$

- The potential V is a function $V : X \rightarrow [0, \infty[$. V is called *simple* if $\forall x \in X, V(x) \in \{0, 1\}$.
- A *well* $x \in X$ is a vertex of G so that $V(x) = 0$. $L = \{1, \dots, j, \dots, N\}$ denotes the set of wells. We assume in what follows that there is no edges between 2 wells. It means that the wells are isolated vertices of G .

2 Dirichlet problems and decay estimates

Let $j \in L$ and $L_j = L \setminus \{j\}$. We will consider the restriction H_j of H to the space of functions $f : X \rightarrow \mathbb{R}$ which vanish on L_j . The ground state of H_j is a function ψ_j which is > 0 on $X \setminus L_j$. We normalize ψ_j by $\psi_j(j) = 1$. The associated eigenvalue is denoted μ_j .

Lemma 1 *As $\hbar \rightarrow 0$, $\lim_{\hbar \rightarrow 0} \psi_j$ is the function ε_j defined by $\varepsilon_j(j) = 1$ and $\varepsilon_j(x) = 0$ if $x \neq j$ and $\lim_{\hbar \rightarrow 0} \mu_j = 0$. Moreover ψ_j and μ_j are analytic functions of \hbar^2 .*

This is clear because the matrix of H_j is analytic in \hbar^2 and the limit for $\hbar = 0$ is a diagonal matrix with all entries > 0 except the j -th which is 0.

Some notations: if $P = (x_0, \dots, x_{|P|})$ is a path, we define the weight $s_\lambda(P)$ by

$$s_\lambda(P) = \hbar^{2|P|} a(x_0) \cdots a(x_{|P|-1})$$

with

$$a(x) = (V(x) - \lambda)^{-1} .$$

Let us note that $s_\lambda(P)$ depends on \hbar . Sometimes it will be convenient to write $s(P) = s_\lambda(P)$.

Theorem 1 *Let us define, for λ close to 0, the function ψ_λ by $\psi_\lambda(j) = 1$, $(\psi_\lambda)|_{L_j} = 0$ and, for $x \notin L$,*

$$\psi_\lambda(x) = \sum_{P: x \rightarrow j} s_\lambda(P) ,$$

where the (convergent) sum is on all paths with $x_0 = x$, $x_{|P|} = j$ and $x_l \notin L$ for $1 \leq l \leq |P| - 1$. Then μ_j is defined implicitly by

$$\sum_{P: j \rightarrow j} s_{\mu_j}(P) = 1 ,$$

where the sum is on all paths with $x_0 = j$, $x_{|P|} = j$ and $x_l \notin L$ for $1 \leq l \leq |P| - 1$.

In particular $\mu_j = \hbar^4 \sum_{y \sim j} V(y)^{-1} + O(\hbar^6)$, $\|\psi_j\| = 1 + O(\hbar^4)$ and

$$\forall x \in X, \psi_j(x) = O(\hbar^{2D(x,j)}) .$$

Remark 1 The implicit equation for μ_j can be expanded as

$$\mu_j = - \sum_{k=2}^{\infty} \hbar^{2k} \sum_{P=(j,x_1,\dots,j), |P|=k} \prod_{l=1}^{|P|-1} (V(x_l) - \mu_j)^{-1} .$$

This equation can be solved induction. This is related to the so-called Rayleigh-Schrödinger series.

Proof.–

The sums on paths are absolutely convergent for \hbar small enough because of the following upper bound:

Lemma 2 If $G = (X, E)$ is a finite graph and $x \in X$, the number of paths of length l starting from x is bounded from above by $(\max_{x \in X} d(x))^l$.

So, for λ close to 0 the series defining ψ is bounded by $O(\sum_l (C\hbar)^{2l})$.

Let us show first that ψ_λ satisfies $((H - \lambda)\psi_\lambda)(x) = 0$ if $x \notin L$.

We have

$$((H - \lambda)\psi_\lambda)(x) = \frac{1}{a(x)}\psi_\lambda(x) - \hbar^2 \sum_{y \sim x, y \notin L_j} \psi_\lambda(y) ,$$

and, using the definition of ψ_λ , the last sum is $\sum_{y \sim x, y \notin L_j} \sum_{Q: y \rightarrow j} s_\lambda(Q)$.

Using the decomposition of $P : x \rightarrow j$ as a path (x, Q) , we get

$$((H - \lambda)\psi_\lambda)(x) = 0 .$$

Similarly we can compute $((H - \lambda)\psi_\lambda)(j)$ as

$$((H - \lambda)\psi_\lambda)(j) = \frac{1}{a(j)} - \hbar^2 \sum_{y \sim x} \sum_{Q: y \rightarrow j} s_\lambda(Q) = \frac{1}{a(j)} \left(1 - \sum_{P: j \rightarrow j} s_\lambda(P) \right) .$$

□

3 The interaction matrix

Our goal is to apply Theorem 3 with \mathcal{F} the space generated by the ψ_j 's with $j \in L$. Using Proposition 1, we can take $\eta = \hbar^4$ and $\varepsilon = \hbar^{2S_0}$ with $S_0 := \min_{i,j \in L, i \neq j} D(i, j)$. The diagonal entries of the interaction matrix H_ε are the μ_j 's estimated in Proposition 1. We need to compute $\langle r_j | \psi_i \rangle$. Using the fact that $((H - \mu_j)\psi_j)(x) = 0$ if $x \notin L \setminus j$, we get $\langle r_j | \psi_i \rangle = \sum_{l \in L \setminus j} ((H - \mu_j)\psi_j)(l)\psi_i(l)$. We have $((H - \mu_j)\psi_j)(l) = \sum_{P:l \rightarrow j} \tilde{s}_{\mu_j}(P)$ with $\tilde{s}_{\mu_j}((l, x_1, \dots, j)) = -\hbar^{2|P|} \prod_{l=1}^{|P|-1} a(x_l)$. We get

$$\langle r_j | \psi_i \rangle = \sum_{P:i \rightarrow j, |P|=S_0} \tilde{s}_{\mu_j}(P) + O(\hbar^{2S_0+2}) .$$

Summarizing, we get the

Theorem 2 *Up to $O(\hbar^{2S_0+2})$, the $|L|$ first eigenvalues of H are those of the matrix $I = \text{Diag}(\mu_j) + r_{ij}$ with*

$$r_{ij} = -\hbar^{2S_0} \sum_{P=(i, x_1, \dots, x_l, \dots, j), |P|=S_0} \prod_{l=1}^{|P|-1} \frac{1}{V(x_l)} ,$$

where the paths P in the sum satisfy $x_l \notin L$ for $1 \leq l \leq |P| - 1$.

4 Simple potentials on graphs of constant degree d

Definition 1 *The potential V is called simple if, for all vertices $x \in X$, we have $V(x) = 0$ or 1.*

If we assume moreover that the vertices of G are all of the same degree d , the matrix I becomes purely combinatorial.

In this case, we have

$$s(P) = \hbar^{2|P|} (-\lambda)^{-1} (1 - \lambda)^{1-|P|} ,$$

and the equation for μ_j is

$$\mu_j = - \sum_{k=2}^{\infty} \hbar^{2k} (1 - \mu_j)^{1-|k|} N_j(k)$$

where $N_j(k)$ is the number of paths $P : j \rightarrow j$ of length k .

The non-diagonal entries of I are given by

$$r_{ij} = -\hbar^{2S_0} \#\{P : i \rightarrow j \mid |P| = S_0\} .$$

5 Application to simulated annealing

The problem is to find the global minimum of a function H on a finite, but large set X . We assume that the set X has a graph structure $G = (X, E)$ which gives a way to move on it.

Example 5.1 X is the set of element of the group \mathcal{S}_N of permutations of N letters. S is a small generating set of \mathcal{S}_N and the G is the associated Cayley graph.

Example 5.2 $X = \{-1, +1\}^Y$ is a spin system on the lattice Y and, if $x, y \in X$, $\{x, y\} \in E$ if all coordinates of x and y are the same except one.

The function H can be assumed to be with values in \mathbb{N} and we can also assume that, for $\{x, y\} \in E$, $H(x) - H(y) = \pm 1$. Let us fix some positive number $T > 0$, the temperature, then there is a probability measure on X , called the Gibbs measure, defined by $\mu_T(\{x\}) = Z^{-1}e^{-H(x)/T}$. As $T \rightarrow 0^+$, the measure μ_T is more and more concentrated on the global minima of H . We can define a Markov process on X by the transition matrix Λ_T defined by $\lambda_{x,y} = 1$ if $H(y) < H(x)$, $\lambda_{x,y} = e^{-(H(y)-H(x))/T}$ if $H(y) > H(x)$ and $\lambda_{x,x} = -\sum_{y \sim x} \lambda_{x,y}$. The quadratic form associated to $-\Lambda_T$ is

$$q_T(f) = \frac{1}{2}Z^{-1} \sum_{x \in X} e^{-H(x)/T} \sum_{y \sim x} \lambda_{x,y} (f(x) - f(y))^2 .$$

The measure μ_T is the stationary measure of this Markov process defined by

$$\text{Prob}(\{\gamma | \gamma(0) = x, \gamma(t) = y\}) = e^{t\Lambda_T^*}(x, y) .$$

The matrix Λ_T gives a symmetric map on $l^2(\mu_T)$ whose eigenvalues are $\lambda_1 = 0 > \lambda_2 \geq \dots$. The speed of convergence of a random trajectory is basically controlled by the gap $-\lambda_2$ of the matrix Λ_T . The main information is given by the asymptotic behavior of the gap as $T \rightarrow 0^+$. This asymptotic behaviour is the main object of the paper [1]. In this paper, we propose an algorithm in order to determine the order of magnitude of the gap: an even power of $\varepsilon = e^{-1/T}$.

The first step is to indentify $l^2(X, \mu_T)$ with $l^2(X, \text{can})$ where can is the measure $\sum_{x \in X} \delta(x)$. This is done using the unitary map $U : l^2(X, \text{can}) \rightarrow l^2(X, \mu_T)$ defined by

$$(Uf)(x) = Z^{\frac{1}{2}} e^{H(x)/2T} f(x) .$$

The quadratic form associated to $H_T = -U^* \Lambda_T U$, $Q_T(f) = q_T(Uf)$ is given by

$$Q_T(f) = \sum_{x \sim y, H(y)=H(x)-1} (f(x) - \varepsilon f(y))^2$$

with $\varepsilon = \exp(-1/2T)$. It can be checked that the lowest eigenvalue of Q_T is 0 with eigenvector $f(x) = \varepsilon^{H(x)}$ which concentrate on the global minimas of H . We have also $H_T = -\varepsilon A_G + V_\varepsilon$ where A_G is the adjacency matrix and $V_\varepsilon(x) = n_+(x) + \varepsilon^2 n_-(x)$ with $n_+(x) = \#\{y \sim x | H(y) = H(x) - 1\}$ and $n_-(x) = \#\{y \sim x | H(y) = H(x) + 1\}$.

Our goal in [1] was do determine the asymptotic behavior of the gap of H_T as $T \rightarrow 0^+$. This can also be done using the previous approach with $\hbar := \sqrt{\varepsilon}$ and V depending now of \hbar in a smooth way.

Appendix A: abstract interaction matrix

Let \mathcal{H} be an Hilbert space (assumed to be real for simplicity) and \mathcal{E}, \mathcal{F} two subspaces of \mathcal{H} , let us define the “distance”

$$d(\mathcal{E}, \mathcal{F}) = \sup_{x \in \mathcal{E}, \|x\|=1} \inf_{y \in \mathcal{F}} \|x - y\| .$$

If $\dim \mathcal{E} = \dim \mathcal{F} = N < \infty$, one checks, using an isometry of \mathcal{H} exchanging \mathcal{E} and \mathcal{F} , that d is symmetric.

Lemma 3 *Let A be self-adjoint on \mathcal{H} , $I = [\alpha, \beta] \subset \mathbb{R}$ and $a > 0$ so that $\text{Spectrum}(A) \cap ([\alpha - a, \alpha] \cup [\beta, \beta + a]) = \emptyset$. Let ψ_j , $j = 1, \dots, N$, so that*

$$\|(A - \mu_j)\psi_j\| \leq \varepsilon \tag{1}$$

with $\alpha \leq \mu_j \leq \beta$ and \mathcal{F} the space generated by the ψ_j 's. If \mathcal{E} is the range of the spectral projector Π of A associated to the interval $I = [\alpha, \beta]$, we have:

$$d(\mathcal{F}, \mathcal{E}) \leq \varepsilon \sqrt{N} / a \sqrt{\lambda_S} ,$$

where λ_S is the smallest eigenvalue of the matrix $S = (s_{ij}) = (\langle \psi_i | \psi_j \rangle)$.

Proof.–

Let $\psi_j = v_j + w_j$ where v_j is the projection of ψ_j on \mathcal{E} . We have, using the fact that w_j belongs to the image of the spectral projector $\text{Id} - \Pi$ and the assumption on the spectrum of A ,

$$\varepsilon \geq \|(A - \mu_j)\psi_j\| \geq \|(A - \mu_j)w_j\| \geq a \|w_j\|$$

and hence $\|\psi_j - v_j\| \leq \varepsilon/a$.

If $\psi = \sum x_j \psi_j$ and $v = \sum x_j v_j$ is the projection of ψ on \mathcal{E} , we have, using Cauchy-Schwarz inequality,

$$\|\psi - v\| \leq \sqrt{\sum x_j^2} \cdot \sqrt{N} \cdot \frac{\varepsilon}{a} ,$$

and:

$$\|\psi\|^2 = \sum x_i x_j s_{i,j} \geq \lambda_S \sum x_j^2 .$$

The result follows. □

We keep the Assumptions of Lemma 3, in particular Equation (1), and assume now that $\dim(\mathcal{E}) = \dim(\mathcal{F}) = N$ so that $d(\mathcal{E}, \mathcal{F}) = 0(\epsilon)$. We assume also that we have two small parameters $\eta = o(1)$, $\epsilon = o(1)$ and that

$$\langle \psi_i | \psi_i \rangle = 1 + O(\eta) \text{ and for } i \neq j, \langle \psi_i | \psi_j \rangle = O(\epsilon) . \quad (2)$$

We denote by $\Psi_i = \psi_i / \|\psi_i\|$, $V_i = \Pi \Psi_i$. If Σ is the matrix of the scalar products $\Sigma = (\langle V_i | V_j \rangle)$ and if (κ_{ij}) denotes the matrix $\Sigma^{-1/2}$, we put $e_i = \sum_k \kappa_{ik} V_k$. The set $\mathcal{O} = \{e_i | i = 1, \dots, N\}$ is an orthonormal basis of \mathcal{E} . The next statement gives an approximation of the matrix of the restriction $A_{\mathcal{E}}$ of A to \mathcal{E} in the basis \mathcal{O} :

Theorem 3 *The matrix $A_{\mathcal{E}}$ of $A|_{\mathcal{E}}$ in the basis \mathcal{O} is given by:*

$$a_{ij} = \langle Ae_i | e_j \rangle = \mu_i \delta_{i,j} + \frac{1}{2} (\langle r_i | \psi_j \rangle + \langle r_j | \psi_i \rangle) + O(\epsilon(\epsilon + \eta)) ,$$

with $r_i = (A - \mu_i) \psi_i = O(\epsilon)$.

Proof. –

First, by Pythagore's Theorem and using Equation (2),

$$\langle V_i | V_j \rangle = \langle \Psi_i | \Psi_j \rangle + O(\epsilon^2) := \delta_{i,j} + T_{i,j}$$

with $T = (T_{ij}) = 0(\epsilon)$.

Similarly

$$\langle AV_i | V_j \rangle = \langle A\Psi_i | \Psi_j \rangle + O(\epsilon^2) :$$

we start with $\Psi_i = V_i + W_i$ and $A\Psi_i = AV_i + AW_i$. Using $A\Psi_i = \mu_i \Psi_i + r_i / \|\psi_i\|$ and projecting on \mathcal{E}^\perp , we get $AW_i = O(\epsilon)$.

We get then using the symmetry of A :

$$(\langle AV_i | V_j \rangle) = D_\mu + \frac{1}{2} (D_\mu T + T D_\mu) + \frac{1}{2} (\langle r_i | \psi_j \rangle + \langle r_j | \psi_i \rangle) + O(\epsilon(\epsilon + \eta)) ,$$

where D_μ is the diagonal matrix whose entries are the μ_i 's.

Using the fact that $(e_i) = (Id - T/2 + O(\epsilon^2))(V_j)$, we get :

$$(\langle Ae_i | e_j \rangle) = (Id - T/2) (\langle AV_i | V_j \rangle) (Id - T/2) + O(\epsilon^2) .$$

The final result follows.

□

Corollary 1 *If $\lambda_1 \leq \dots \leq \lambda_N$ are the eigenvalues of A in the interval I and $\mu_1 \leq \dots \leq \mu_N$ are the eigenvalues of*

$$D_\mu + \frac{1}{2} (\langle r_i | \psi_j \rangle + \langle r_j | \psi_i \rangle) ,$$

then

$$\lambda_j = \mu_j + O(\varepsilon(\varepsilon + \eta)) .$$

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