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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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- $\Delta$  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  $\psi_j$  which is  $> 0$  on  $X \setminus L_j$ . We normalize  $\psi_j$  by  $\psi_j(j) = 1$ . The associated eigenvalue is denoted  $\mu_j$ .

**Lemma 1** *As  $\hbar \rightarrow 0$ ,  $\lim_{\hbar \rightarrow 0} \psi_j$  is the function  $\varepsilon_j$  defined by  $\varepsilon_j(j) = 1$  and  $\varepsilon_j(x) = 0$  if  $x \neq j$  and  $\lim_{\hbar \rightarrow 0} \mu_j = 0$ . Moreover  $\psi_j$  and  $\mu_j$  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  $\lambda$  close to 0, the function  $\psi_\lambda$  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  $\mu_j$  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  $\mu_j$  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  $\lambda$  close to 0 the series defining  $\psi$  is bounded by  $O(\sum_l (C\hbar)^{2l})$ .

Let us show first that  $\psi_\lambda$  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  $\psi_\lambda$ , 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  $\psi_j$ '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  $H_\varepsilon$  are the  $\mu_j$ '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*

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

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  $\mu_j$  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  $\mu_T$  is more and more concentrated on the global minima of  $H$ . We can define a Markov process on  $X$  by the transition matrix  $\Lambda_T$  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  $\mu_T$  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  $\Lambda_T$  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  $\Lambda_T$ . 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  $\psi_j$ ,  $j = 1, \dots, N$ , 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  $\psi_j$ 's. If  $\mathcal{E}$  is the range of the spectral projector  $\Pi$  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  $\lambda_S$  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  $\psi_j$  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  $\psi$  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  $\Sigma$  is the matrix of the scalar products  $\Sigma = (\langle V_i | V_j \rangle)$  and if  $(\kappa_{ij})$  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  $D_\mu$  is the diagonal matrix whose entries are the  $\mu_i$ '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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