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

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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

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

where

- $h$ is a positive parameter. The semi-classical limit that we will study is $h \to 0$.

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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 $V : X \to [0, \infty[$. $V$ 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 $V(x) = 0$. $L = \{1, \cdots, j, \cdots, N\}$ 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 $f : X \to \mathbb{R}$ 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 $h \to 0$, $\lim_{h \to 0} \psi_j$ is the function $\varepsilon_j$ defined by $\varepsilon_j(j) = 1$ and $\varepsilon_j(x) = 0$ is $x \neq j$ and $\lim_{h \to 0} \mu_j = 0$. Moreover $\psi_j$ and $\mu_j$ are analytic functions of $h^2$.

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

Some notations: if $P = (x_0, \cdots, x_{|P|})$ is a path, we define the weight $s_\lambda(P)$ by
  \[
  s_\lambda(P) = h^{2|P|} a(x_0) \cdots a(x_{|P|-1})
  \]
with
  \[
  a(x) = (V(x) - \lambda)^{-1}.
  \]

Let us note that $s_\lambda(P)$ depends on $h$. 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 $x \notin L$,
  \[
  \psi_\lambda(x) = \sum_{P : x \to j} s_\lambda(P),
  \]
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 implicitely by
  \[
  \sum_{P : j \to j} s_{\mu_j}(P) = 1,
  \]
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 $\mu_j = h^4 \sum_{y} V(y)^{-1} + O(h^6)$, $\|\psi_j\| = 1 + O(h^4)$ and

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

**Remark 1** The implicit equation for $\mu_j$ can be expanded as

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

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 $h$ 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 $O(\sum_l (Ch)^{2l})$.

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

We have

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

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

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

$\square$
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 $H_\mathcal{F}$ 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 $((H - \mu_j)\psi_j)(l) = \sum_{P : j \rightarrow l} \bar{s}_{\mu_j}(P) \psi_i(l)$. We get

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

Summarizing, we get the

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

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

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

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

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

$$r_{ij} = -\hbar^{2S_0} \#\{P : i \rightarrow j | P = S_0\}.$$
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 elements of the group $S_N$ of permutations of $N$ letters. $S$ is a small generating set of $S_N$ 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 $\mathbb{R}$ 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 $\mu_T(\{x\}) = \frac{1}{Z} e^{-H(x)/T}$. As $T \to 0^+$, 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

$$
\lambda_{x,y} = 1 \text{ if } H(y) < H(x), \\
\lambda_{x,y} = e^{-H(y) - H(x)/T} \frac{1}{Z} e^{-H(x)/T} \text{ if } H(y) > H(x), \\
\lambda_{x,x} = -\sum_{y \sim x} \lambda_{x,y}.
$$

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 $\lambda_1 = 0 > \lambda_2 \geq \cdots$. 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 $T \to 0^+$. 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 $U : l^2(X, \text{can}) \to l^2(X, \mu_T)$ defined by

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

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 \( \epsilon = \exp(-1/2T) \). It can be checked that the lowest eigenvalue of \( Q_T \) is 0 with eigenvector \( f(x) = \epsilon^H(x) \) which concentrate on the global minimas of \( H \). We have also \( H_T = -\epsilon A_G + V_\epsilon \) where \( A_G \) is the adjacency matrix and \( V_\epsilon(x) = n_+(x) + \epsilon^2 n_-(x) \) 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 to determine the asymptotic behavior of the gap of \( H_T \) as \( T \to 0^+ \). This can also be done using the previous approach with \( h := \sqrt{\epsilon} \) and \( V \) depending now of \( h \) 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 \( \psi_j, j = 1, ..., N \), so that

\[
\| (A - \mu_j) \psi_j \| \leq \epsilon \quad (1)
\]

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:

\[
d(\mathcal{F}, \mathcal{E}) \leq \epsilon \sqrt{N/a} \sqrt{\lambda_S},
\]

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 \( A \),

\[
\epsilon \geq \| (A - \mu_j) \psi_j \| \geq \| (A - \mu_j) w_j \| \geq a \| w_j \|
\]

and hence \( \| \psi_j - v_j \| \leq \epsilon/a \).

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,

\[
\| \psi - v \| \leq \sqrt{\sum x_j^2 \sqrt{N} \frac{\epsilon}{a}},
\]

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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 \( d(\mathcal{E}, \mathcal{F}) = o(\epsilon) \). We assume also that we have two small parameters \( \eta = o(1), \epsilon = o(1) \) and that
\[ \langle \psi_i | \psi_i \rangle = 1 + O(\eta) \text{ and for } i \neq j, \langle \psi_i | \psi_j \rangle = O(\epsilon). \] (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 \( \mathcal{O} = \{ e_i | i = 1, \cdots, N \} \) 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:
\[ a_{ij} = \langle A e_i | e_j \rangle = \mu_i \delta_{i,j} + \frac{1}{2} (\langle r_i | \psi_j \rangle + \langle r_j | \psi_i \rangle) + O(\epsilon(\epsilon + \eta)) \],
with \( r_i = (A - \mu_i) \psi_i = O(\epsilon) \).

**Proof.** –

First, by Pythagore’s Theorem and using Equation (2),
\[ \langle V_i | V_j \rangle = \langle \Psi_i | \Psi_j \rangle + O(\epsilon^2) := \delta_{i,j} + T_{ij} \]
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 \( (e_i) = (\text{Id} - T/2 + O(\epsilon^2)) (V_j) \), we get :
\[ \langle A e_i | e_j \rangle = (\text{Id} - T/2) (\langle AV_i | V_j \rangle) (\text{Id} - T/2) + O(\epsilon^2) \].
The final result follows.
Corollary 1 If $\lambda_1 \leq \cdots \leq \lambda_N$ are the eigenvalues of $A$ in the interval $I$ and $\mu_1 \leq \cdots \leq \mu_N$ are the eigenvalues of

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

then

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

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