

# Semiclassical analysis for a Schrödinger operator with a U(2) artificial gauge: the periodic case

Abderemane Morame, Francoise Truc

#### ▶ To cite this version:

Abderemane Morame, Francoise Truc. Semiclassical analysis for a Schrödinger operator with a U(2) artificial gauge: the periodic case. IF\_PREPUB. 2014. <a href="https://doi.org/10.1009/s6313v2">https://doi.org/10.1009/s6313v2</a>>

## HAL Id: hal-00936313

https://hal.archives-ouvertes.fr/hal-00936313v2

Submitted on 24 Jun 2014

**HAL** is a multi-disciplinary open access archive for the deposit and dissemination of scientific research documents, whether they are published or not. The documents may come from teaching and research institutions in France or abroad, or from public or private research centers. L'archive ouverte pluridisciplinaire **HAL**, est destinée au dépôt et à la diffusion de documents scientifiques de niveau recherche, publiés ou non, émanant des établissements d'enseignement et de recherche français ou étrangers, des laboratoires publics ou privés.

# Semiclassical analysis for a Schrödinger operator with a U(2) artificial gauge: the periodic case

## A. Morame<sup>1</sup> and F. $Truc^2$ June 16, 2014

Université de Nantes, Faculté des Sciences, Dpt. Mathématiques,
 UMR 6629 du CNRS, B.P. 99208, 44322 Nantes Cedex 3, (FRANCE),
 E.Mail: Abderemane.Morame@univ-nantes.fr
 Université de Grenoble I, Institut Fourier,
 UMR 5582 CNRS-UJF, B.P. 74,
 38402 St Martin d'Hères Cedex, (France),
 E.Mail: Francoise.Truc@ujf-grenoble.fr

#### Abstract

We consider a Schrödinger operator with a Hermitian 2x2 matrix-valued potential which is lattice periodic and can be diagonalized smoothly on the whole  $\mathbb{R}^n$ . In the case of potential taking its minimum only on the lattice, we prove that the well-known semiclassical asymptotic of first band spectrum for a scalar potential remains valid for our model.

**Keywords:** semiclassical asymptotic, spectrum, eigenvalues, Schrodinger, periodic potential, BKW method, width of the first band, magnetic field. **AMS MSC 2000:** 35J10, 35P15, 47A10, 81Q10, 81Q20.

## Contents

1	Introduction	2
2	Preliminary: the artificial gauge model	3
3	Proof of Theorem 2.1	5
4	Asymptotic of the first band	7
5	B.K.W. method for the Dirichlet ground state	11

## 1 Introduction

Schrödinger operators with periodic matrix-valued potentials appear in many models in physics. Such models have been used recently to describe the motion of an atom in optical fields ([Co], [Co-Da], [Da-al]), see also [Ca-Yu]. The aim of this paper is to investigate their spectral properties using semiclassical analysis. We focus on the first spectral band and assume that the potential has a non degenerate minimum. The Schrödinger operators with a non-Abelian gauge potential are Hamiltonian operators on  $L^2(\mathbb{R}^n; \mathbb{C}^m)$  of the following form:

$$H^{h} = h^{2} \sum_{k=1}^{n} (D_{x_{k}} I - A_{k})^{2} + V + hQ + h^{2} R = P^{h}(x, hD) . \tag{1.1}$$

The classical symbol of  $P^h(x, hD)$ ,  $P^h(x, \xi)$ , for  $(x, \xi) \in \mathbb{R}^n \times \mathbb{R}^n$ , is given by

$$P^{h}(x,\xi) = \sum_{k=1}^{n} \left\{ (\xi_{k}I - hA_{k}(x))^{2} + ih^{2}\partial_{x_{k}}A_{k}(x) \right\} + V(x) + hQ(x) + h^{2}R(x) ,$$
(1.2)

I is the identity  $m \times m$  matrix, V, Q, R and the  $A_k$  are hermitian  $m \times m$  matrix with smooth coefficients and  $\Gamma$  periodic:

$$A_{k} = (a_{k,ij}(x))_{1 \leq i,j \leq m}, \quad V = (v_{ij}(x))_{1 \leq i,j \leq m}, 
Q = (q_{ij}(x))_{1 \leq i,j \leq m}, \quad R = (r_{ij}(x))_{1 \leq i,j \leq m}, 
a_{k,ij}, v_{ij}, q_{ij}, r_{ij} \in C^{\infty}(\mathbb{R}^{n}; \mathbb{C}), 
\overline{a_{k,ji}} = a_{k,ij}, \overline{v_{ji}} = v_{ij}, \overline{q_{ji}} = q_{ij}, \overline{r_{ji}} = r_{ij} 
a_{k,ij}(x - \gamma) = a_{k,ij}(x), v_{ij}(x - \gamma) = v_{ij}(x), 
q_{ij}(x - \gamma) = q_{ij}(x) \text{ and } r_{ij}(x - \gamma) = r_{ij}(x) \quad \forall \gamma \in \Gamma;$$

$$(1.3)$$

 $\Gamma$  is a lattice of  $\mathbb{R}^n$ ,  $\Gamma = \{\sum_{k=1}^n m_k \beta_k; \ m_k \in \mathbb{Z}\},$ 

 $\beta_1, \beta_2, \ldots, \beta_n \in \mathbb{R}^n$  form a basis,  $det(\beta_1, \beta_2, \ldots, \beta_n) \neq 0$ . We use the notation  $D = (D_{x_1}, \ldots, D_{x_n})$  where  $D_{x_k} = -i\partial_{x_k}$ , k = 1...n, so  $D^2 = -\Delta$  is the Laplacian operator on  $L^2(\mathbb{R}^n)$ .

The dual basis  $\{\beta_1^{\star}, \dots, \beta_n^{\star}\}$  of the reciprocal lattice  $\Gamma^{\star}$ , is the basis of  $\mathbb{R}^n$  defined by the relations

$$\beta_j^{\star}.\beta_k = 2\pi\delta_{jk} : \Gamma^{\star} = \{\sum_{k=1}^n m_k \beta_k^{\star}; m_k \in \mathbb{Z}\}.$$

The fundamental cell, the Wigner-Seitz cell,

$$\mathbb{W}^n = \{ \sum_{k=1}^n x_k \beta_k \; ; \; x_k \in ] - \frac{1}{2}, \frac{1}{2} [ \} \; ,$$

will be identified with the n-dimensional torus  $\mathbb{T}^n = \mathbb{R}^n/\Gamma$  and the dual cell, the Brillouin zone, is defined by

$$\mathbb{B}^{n} = \{ \sum_{k=1}^{n} \theta_{k} \beta_{k}^{\star}; \theta_{k} \in ] - \frac{1}{2}, -\frac{1}{2} [ \} .$$

We will identify  $L^2(\mathbb{T}^n;\mathbb{C}^m)$  with  $\Gamma$  periodic functions of  $L^2_{loc}(\mathbb{R}^n;\mathbb{C}^m)$  provided with the norm of  $L^2(\mathbb{W}^n;\mathbb{C}^m)$ . In the same way the Sobolev space  $W^k(\mathbb{T}^n;\mathbb{C}^m)$ , with  $k \in \mathbb{N}$ , may be identified with  $\Gamma$  periodic functions of  $W_{loc}^k(\mathbb{R}^n; \mathbb{C}^m)$  provided with the norm of  $W^k(\mathbb{W}^n; \mathbb{C}^m)$ .

By Floquet theory, (see [Ea] or [Re-Si]), we have

$$H^h = \int_{\mathbb{R}^n}^{\oplus} H^{h,\theta} d\theta ,$$

with  $H^{h,\theta}$  the partial differential operator  $P_h(x,h(D-\theta))$  on  $L^2(\mathbb{T}^n;\mathbb{C}^m)$ The ellipticity of  $P_h(x, h(D-\theta))$  implies that the spectrum of  $H^{h,\theta}$  is discrete

$$\operatorname{sp}(H^{h,\theta}) = \{\lambda_i^{h,\theta}; \ j \in \mathbb{N}^*\}, \ \lambda_1^{h,\theta} \le \lambda_2^{h,\theta} \le \dots \le \lambda_i^{h,\theta} \le \lambda_{i+1}^{h,\theta} \le \dots$$
 (1.4)

each  $\lambda_j^{h,\theta}$  is an eigenvalue of finite multiplicity and each eigenvalue is repeated according to its multiplicity.

(When m=1 and  $V=Q=R=A_k=0$ ,  $(\frac{1}{\sqrt{|\mathbb{T}^n|}}e^{i\omega x})_{\omega\in\Gamma^*}$  is the Hilbert basis of  $L^2(\mathbb{T}^n)$  which is composed of eigenfunctions of  $h^2(D-\theta)^2$ ).

The Floquet theory guarantees that

$$\operatorname{sp}(H^h) = \bigcup_{\theta \in \mathbb{R}^n} \operatorname{sp}(H^{h,\theta}) = \bigcup_{j=1}^{\infty} b_j^h,$$
(1.5)

where  $b_j^h$  denotes the j-th band  $b_j^h = \{\lambda_j^{h,\theta}, \theta \in \mathbb{B}^n\}$ . In the sequel  $h_0$  will be a non negative small constant, h will be in  $]0, h_0[$ , and any non negative constant which doesn't depend on h will invariably be denoted by C.

#### Preliminary: the artificial gauge model 2

We will be interested in the model of artificial gauge considered in [Co], [Co-Da] and [Da-al]

$$m = 2, \ V = vI + W, \ A_k = Q = R = 0, \ \forall k, \ W = w.\sigma, \text{ with } w = (w_1, w_2, w_3), \ v \text{ and the } w_j \text{ are in } C^{\infty}(\mathbb{R}^n; \mathbb{R}),$$
 (2.1)

we denote  $\sigma = (\sigma_1, \sigma_2, \sigma_3)$ , where the  $\sigma_i$  are the Pauli matrices.

Let us remark that

$$V = vI + W, \quad W = w.\sigma, \quad W^2 = |w|^2 I.$$
 (2.2)

In the sequel we will assume that

$$|w| > 0$$
  
  $v(x) - |w(x)|$  has a unique non degenerate minimum on  $\mathbb{T}^n$ . (2.3)

Due to the invariance of the Laplacian by translation and by the action of  $\mathbb{O}(n)$ , we can assume, up to a composition by a translation of the potentials, that

$$v(\gamma) - |w(\gamma)| < v(x) - |w(x)|, \ \forall x \in \mathbb{R}^n \setminus \Gamma \text{ and } \forall \gamma \in \Gamma,$$

$$v(x) - |w(x)| = E_0 + \sum_{k=1}^n \tau_k^2 x_k^2 + \mathbf{O}(|x|^3), \text{ as } |x| \to 0,$$

$$(2.4)$$

 $(\tau_k > 0, \ \forall k).$ 

There exists  $U \in \mathbb{U}(2)$ , (a unitary  $2 \times 2$  matrix), such that

$$U^{\star}VU = \widetilde{V} = \begin{bmatrix} v - |w| & 0\\ 0 & v + |w| \end{bmatrix} . \tag{2.5}$$

As |w| never vanishes, U = U(x) can be chosen smooth and  $\Gamma$  periodic:

$$U = \begin{pmatrix} u_{11} & u_{12} \\ u_{21} & u_{22} \end{pmatrix} \in C^{\infty}(\mathbb{T}^n; \mathbb{U}(2));$$

for example 
$$u_{11} = \frac{1}{2\sqrt{|w|(|w| - \text{Re}((w_1 + iw_2)e^{-i\theta}))}}(w_3 - |w| + e^{i\theta}(w_1 - iw_2)),$$

$$u_{21} = \frac{1}{2\sqrt{|w|(|w| - \operatorname{Re}(w_1 + iw_2)e^{-i\theta})}} (w_1 + iw_2 - e^{i\theta}(w_3 + |w|)),$$

$$u_{12} = \overline{u_{21}}, \ u_{22} = -\overline{u_{11}} \text{ and } \theta = \chi(\frac{w_2^2 + w_3^2}{|w|^2})\frac{\pi}{2},$$

where  $\chi(t)$  is a smooth function on the real line,  $0 \le \chi(t) \le 1$ ,

 $\chi(t) = 1$  when  $|t| \le 1/4$  and  $\chi(t) = 0$  when  $|t| \ge 1/2$ . So

$$U = (\alpha, \beta, \rho) \cdot \sigma + i\delta\sigma_0, \quad \text{with } (\alpha, \beta, \rho, \delta) \in C^{\infty}(\mathbb{T}^n; \mathbb{S}^3);$$
 (2.6)

 $\sigma_0$  is the 2 × 2 identity matrix and  $\mathbb{S}^3$  is the unit sphere of  $\mathbb{R}^4$ .

When  $w_1 + iw_2 \neq 0$  or when  $w_3 < 0$ , one can choose U such that  $\delta = 0$  by taking  $(\alpha, \beta, \rho) = \frac{1}{\sqrt{2|w|}} \left(-\frac{w_1}{\sqrt{|w| - w_3}}, -\frac{w_2}{\sqrt{|w| - w_3}}, \sqrt{|w| - w_3}\right)$ .

Firstly let us expand the formula of the operator

$$\widetilde{H}^{h} = U^{\star}H^{h}U = h^{2}D^{2}I + U^{\star}VU - 2ih^{2}\sum_{k=1}^{n} \left[ (U^{\star}\partial_{x_{k}}U)D_{x_{k}} - h^{2}U^{\star}\partial_{x_{k}}^{2}U \right]$$

which can be rewritten as

$$\widetilde{H}^h = U^* H^h U = h^2 \sum_{k=1}^n (D_{x_k} I - A_k)^2 + \widetilde{V} + h^2 R,$$
 (2.7)

where  $A_k = iU^*\partial_{x_k}U$ :

$$A_{k} = [(\partial_{x_{k}}\alpha, \partial_{x_{k}}\beta, \partial_{x_{k}}\rho) \wedge (\alpha, \beta, \rho) + (\delta\partial_{x_{k}}\alpha - \alpha\partial_{x_{k}}\delta, \delta\partial_{x_{k}}\beta - \beta\partial_{x_{k}}\delta, \delta\partial_{x_{k}}\rho - \rho\partial_{x_{k}}\delta)].\sigma,$$
(2.8)

and

$$R = \sum_{k=1}^{n} \left\{ (U^* \partial_{x_k} U)^2 + (\partial_{x_k} U^*) \cdot (\partial_{x_k} U) \right\}.$$
 (2.9)

So we can assume that  $H^h$  is of the form (1.1) with  $m=2,\ Q=0,\ A_k$  and R given by (2.8) and (2.9), with U defined by (2.6), and  $V=\widetilde{V}$  a diagonal matrix given by (2.5).

**Theorem 2.1** Under the above assumptions, the first bands  $b_j^h$ , j = 1, 2, ..., of  $H^h$  are concentrated around the value  $h\mu_j + E_0$  j = 1, 2, ..., in the sense that, there exist  $N_0 > 1$  and  $h_0 > 0$  such that

$$distance(h\mu_j + E_0, b_j^h) \le Ch^2$$
,  $\forall j < N_0 \text{ and } \forall h, \ 0 < h < h_0$ ,

where  $\mu_j = \sum_{k=1}^n (2j_k + 1)\tau_k$ ,  $j_k \in \mathbb{N}$ , the  $(\mu_\ell)_{\ell \in \mathbb{N}^*}$  is the increasing sequence of the

eigenvalues of the harmonic oscillator  $-\Delta + \sum_{k=1}^{n} \tau_k^2 x_k^2$ .

## 3 Proof of Theorem 2.1

*Proof.* According to the above discussion, we can assume that

$$H^h = P^h(x, hD)$$
, with  $P^h(x, hD) = \begin{pmatrix} P_{11}^h(x, hD) & P_{12}^h(x, hD) \\ P_{21}^h(x, hD) & P_{22}^h(x, hD) \end{pmatrix}$ , (3.1)

with

$$P_{11}^{h}(x, hD) = h^{2}(D - a_{.,11}(x))^{2} + v(x) - |w(x)| + h^{2}r_{11}(x)$$

$$P_{22}^{h}(x, hD) = h^{2}(D + a_{.,11}(x))^{2} + v(x) + |w(x)| + h^{2}r_{22}(x)$$

$$P_{12}^{h}(x, hD) = -h^{2}a_{.,12}(x).(D + a_{.,11}(x)) - h^{2}a_{.,12}(x).(D - a_{.,11}(x))$$

$$+ ih^{2}div(a_{.,12}(x)) + h^{2}r_{12}(x)$$

$$P_{21}^{h}(x, hD) = -h^{2}a_{.,21}(x)(D - a_{.,11}(x)) - h^{2}a_{.,21}(x).(D + a_{.,11}(x))$$

$$+ ih^{2}div(a_{.,21}(x)) + h^{2}r_{21}(x).$$

$$(3.2)$$

 $(D = (D_{x_1}, D_{x_2}, \dots, D_{x_n}) \text{ and } a_{.,ij}(x) = (a_{1,ij}(x), a_{2,ij}(x), \dots, a_{n,ij}(x)).)$ (We used that  $a_{.,22} = -a_{.,11}$ ).

Let us denote by  $H_{11}^{h,\theta}$  and  $H_{22}^{h,\theta}$  the operators associated with  $P_{11}^h(x,h(D-\theta))$  and  $P_{22}^h(x,h(D-\theta))$  on  $L^2(\mathbb{T}^n;\mathbb{C})$ . Then, if  $c_0 = \min |w(x)|$  and  $c_1 = \max |R(x)|$ ,

$$\operatorname{sp}(H_{11}^{h,\theta}) \subset [E_0 - h^2 c_1, +\infty[ \text{ and } \operatorname{sp}(H_{22}^{h,\theta}) \subset [E_0 - h^2 c_1 + 2c_0, +\infty[.$$

To prove the theorem it is then enough to prove the proposition below.

**Proposition 3.1** Let us consider a constant c,  $0 < c < c_0$ . Then there exists  $C_0 > 0$  such that, for any  $E^h \in ]-\infty, E_0 + 2c[$ , we have

$$E^{h} \in \operatorname{sp}(H^{h,\theta}) \Rightarrow \operatorname{distance}(E^{h}, \operatorname{sp}(H^{h,\theta}_{11}) \leq C_{0}h^{2}$$

$$E^{h} \in \operatorname{sp}(H^{h,\theta}_{11}) \Rightarrow \operatorname{distance}(E^{h}, \operatorname{sp}(H^{h,\theta})) \leq C_{0}h^{2}.$$

$$(3.3)$$

Proof. For such  $E^h$ ,  $(H_{22}^{h,\theta} - E^h)^{-1}$  exists and, thanks to semiclassical pseudodifferential calculus of [Ro] (see also [Di-Sj] ), for  $h_0 > 0$  small, if  $0 < h < h_0$  then  $\|(H_{22}^{h,\theta} - E^h)^{-1}\|_{L^2(\mathbb{T}^n)} + \|h(D - \theta)(H_{22}^{h,\theta} - E^h)^{-1}\|_{L^2(\mathbb{T}^n)} + \|(H_{22}^{h,\theta} - E^h)^{-1}h(D - \theta)\|_{L^2(\mathbb{T}^n)} + \|h(D - \theta)(H_{22}^{h,\theta} - E^h)^{-1}h(D - \theta)\|_{L^2(\mathbb{T}^n)} \le C$ , and then

$$||P_{12}^h(x,h(D-\theta))(H_{22}^{h,\theta}-E^h)^{-1}P_{21}^h(x,h(D-\theta))||_{L^2(\mathbb{T}^n)} \le h^2C.$$

So if  $E^h \in \operatorname{sp}(H^{h,\theta})$ , then  $u^h = (u_1^h, u_2^h) \neq (0,0)$  is an eigenfunction of  $H^{h,\theta}$  associated with  $E^h$  iff

$$H_{11}^{h,\theta}u_1^h + P_{12}^h(x, h(D-\theta))u_2^h = E^h u_1^h u_2^h = -(H_{22}^{h,\theta} - E^h I)^{-1} P_{21}^h(x, h(D-\theta))u_1^h.$$
(3.4)

In fact  $E^h \in ]-\infty, E_0 + c[$  will be an eigenvalue of  $H^{h,\theta}$  iff there exists  $u_1^h$  in the Sobolev space  $W^2(\mathbb{T}^n;\mathbb{C}), \|u_1^h\|_{L^2(\mathbb{T}^n)} \neq 0$ , such that

$$H_{11}^{h,\theta}u_1^h - P_{12}^h(x,h(D-\theta))(H_{22}^{h,\theta} - E^hI)^{-1}P_{21}^h(x,h(D-\theta))u_1^h = E^hu_1^h,$$

then we get the first part of Proposition 3.1.

If  $E^h$  is an eigenvalue of  $H_{11}^{h,\theta}$  satisfying the assumption of Proposition 3.1, and  $u_1^h$  an associated eigenfunction, then with  $u^h = (u_1^h, -(H_{22}^{h,\theta} - E^h)^{-1}P_{21}^h(x, h(D - \theta))u_1^h)$ , one has

$$\begin{aligned} &\|(H^{h,\theta} - E^h I)u^h\|_{L^2(\mathbb{T}^n;\mathbb{C}^2)} \\ &= \|P_{12}^h(x, h(D-\theta))(H_{22}^{h,\theta} - E^h)^{-1}P_{21}^h(x, h(D-\theta))u_1^h\|_{L^2(\mathbb{T}^n;\mathbb{C})} \\ &\leq h^2 C\|u^h\|_{L^2(\mathbb{T}^n;\mathbb{C}^2)} \,, \end{aligned}$$

we get the second part of Proposition 3.1.

Theorem 2.1 follows from Proposition 3.1 and [Si-1], [Si-2], [He-Sj-1] and [He-Sj-2] results, (see also [He]), which guarantee that the sequence of eigenvalues of  $H_{11}^{h,\theta}$ ,  $(\lambda_j(H_{11}^{h,\theta}))_{j\in\mathbb{N}^*}$  satisfies  $\forall N_0>1,\ \exists h_0>0,\ C_0>0\ s.t.\ \forall h,\ 0< h< h_0$  and  $\forall j\leq N_0$ ,  $|\lambda_j(H_{11}^{h,\theta})-(h\mu_j^h+E_0)|\leq C_0h^2\square$ 

## 4 Asymptotic of the first band

For any real Lipschitz  $\Gamma$  periodic function  $\phi$ , and for any  $u \in W^2(\mathbb{T}^n; \mathbb{C}^2)$ , we have the identity

$$\operatorname{Re}_{k=1} \left( \langle P^{h}(x, h(D-\theta))u | e^{2\phi/h}u \rangle_{L^{2}(\mathbb{T}^{n};\mathbb{C}^{2})} \right) = \sum_{k=1}^{n} h^{2} \| ((D_{x_{k}} - \theta_{k})I - A_{k})e^{\phi/h}u \|_{L^{2}(\mathbb{T}^{n};\mathbb{C}^{2})}^{2} + \langle (\widetilde{V} - |\nabla\phi|^{2}I + h^{2}R)u | e^{2\phi/h}u \rangle_{L^{2}(\mathbb{T}^{n};\mathbb{C}^{2})} .$$

$$(4.1)$$

This identity enables us to apply the method used in [He-Sj-1], (see also [He] and [Ou]). We define the Agmon [Ag] distance on  $\mathbb{R}^n$ 

$$d(y,x) = \inf_{\gamma} \int_{0}^{1} \sqrt{v(\gamma(t)) - |w(\gamma(t))| - E_{0}| \dot{\gamma}(t)| dt}, \qquad (4.2)$$

the inf is taken among paths such that  $\gamma(0) = y$  and  $\gamma(1) = x$ .

For common properties of the Agmon distance, one can see for example [Hi-Si].

We will use that, for any fixed  $y \in \mathbb{R}^n$ , the function d(y,x) is a Lipschitz function on  $\mathbb{R}^n$  and  $|\nabla_x d(y,x)|^2 \le v(x) - |w(x)| - E_0$  almost everywhere on  $\mathbb{R}^n$ .

Using that the zeros of  $v(x) - w(x) - E_0$  are the elements of  $\Gamma$  and are non degenerate, we get that the real function  $d_0(x) = d(0, x)$  satisfies, (see [He-Sj-1]),  $|\nabla d_0(x)|^2 = v(x) - |w(x)| - E_0$  in a neighbourhood of 0.

We summarize the properties of the Agmon distance we will need:

i) 
$$\exists R_0 > 0 \text{ s.t. } d_0(x) \in C^{\infty}(B_0(R_0))$$
  
ii)  $|\nabla d_0(x)|^2 = v(x) - |w(x)| - E_0$ ,  $\forall x \in B_0(R_0)$   
iii)  $|\nabla d_0(x)|^2 \le v(x) - |w(x)| - E_0$   
iv)  $|\nabla d_{\Gamma}(x)|^2 \le v(x) - |w(x)| - E_0$ 

$$(4.3)$$

where  $d_0(x) = d(0, x), \ B_0(r) = \{x \in \mathbb{R}^n; \ d_0(x) < r\}$ and  $d_{\Gamma}(x) = d(\Gamma, x) = \min_{\omega \in \Gamma} d(\omega, x).$ 

The least Agmon distance in  $\Gamma$  is

$$S_0 = \inf_{1 \le k \le n} d_0(\beta_k) = \inf_{\rho \ne \omega, \ (\omega, \rho) \in \Gamma^2} d(\omega, \rho) \ . \tag{4.4}$$

The Agmon distance on  $\mathbb{T}^n$ ,  $d^{\mathbb{T}^n}(.,.)$ , is defined by its  $\Gamma$ -periodic extension on  $(\mathbb{R}^n)^2$ 

$$d^{\mathbb{T}^n}(y,x) = \min_{\omega \in \Gamma} d(y,x+\omega).$$

Then

$$\frac{S_0}{2} = \sup_{r} \{r > 0 \text{ s.t. } \{x \in \mathbb{T}^n; \ d^{\mathbb{T}^n}(x_0, x) < r\} \text{ is simply connected} \}, \qquad (4.5)$$

where  $x_0$  is the single point in  $\mathbb{T}^n$  such that  $v(x_0) - |w(x_0)| = E_0$ . The  $\Gamma$ -periodic function on  $\mathbb{R}^n$ ,  $d_{\Gamma}(x)$  is the one corresponding to the extension of  $d^{\mathbb{T}^n}(x_0, x)$ .

If  $\lambda^{h,\theta}$  is an eigenvalue of  $H^{h,\theta}$  and if  $u^{h,\theta}$  is an associated eigenfunction, then by (4.1) one gets as in the scalar case considered in [He-Sj-1]) and [He-Sj-2],

$$\sum_{k=1}^{n} h^{2} \| ((D_{x_{k}} - \theta_{k})I - A_{k})e^{\phi/h}u^{h,\theta} \|_{L^{2}(\mathbb{T}^{n};\mathbb{C}^{2})}^{2} \\
+ < [\widetilde{V} - |\nabla\phi|^{2}I + h^{2}R - \lambda^{h,\theta}I]_{+}u^{h,\theta} | e^{2\phi/h}u^{h,\theta} >_{L^{2}(\mathbb{T}^{n};\mathbb{C}^{2})} \\
= < [\widetilde{V} - |\nabla\phi|^{2}I + h^{2}R - \lambda^{h,\theta}I]_{-}u^{h,\theta} | e^{2\phi/h}u^{h,\theta} >_{L^{2}(\mathbb{T}^{n};\mathbb{C}^{2})}, \tag{4.6}$$

so, when  $\phi(x) = d^{\mathbb{T}^n}(x_0, x)$ , necessarily  $\lambda^{h,\theta} - E_0 + \mathbf{O}(h^2) > 0$ , and if  $h/C < \lambda^{h,\theta} - E_0 < hC$ , then  $u^{h,\theta}$  is localized in energy near  $x_0$ , for any  $\eta \in ]0,1[, \exists C_{\eta} > 0$  such that

$$\sum_{k=1}^{n} h^{2} \| ((D_{x_{k}} - \theta_{k})I - A_{k}) e^{\eta d^{\mathbb{T}^{n}}(x_{0}, x)/h} u^{h, \theta} \|_{L^{2}(\mathbb{T}^{n}; \mathbb{C}^{2})}^{2} \\
+ (1 - \eta^{2}) < (v - |w| - E_{0}) u^{h, \theta} |e^{2\eta d^{\mathbb{T}^{n}}(x_{0}, x)/h} u^{h, \theta} >_{L^{2}(\mathbb{T}^{n}; \mathbb{C}^{2})}^{2} \\
\leq h C_{\eta} \int_{\{x \in \mathbb{T}^{n}; d^{\mathbb{T}^{n}}(x_{0}, x) < \sqrt{h}C\}} |u^{h, \theta}(x)|^{2} dx.$$
(4.7)

Let  $\Omega \subset \mathbb{T}^n$  an open and simply connected set with smooth boundary satisfying, for some  $\eta$ ,  $0 < \eta < S_0/2$ ,

$$\{x \in \mathbb{T}^n; \ d^{\mathbb{T}^n}(x_0, x) < \frac{S_0 - \eta}{2}\} \subset \Omega \subset \{x \in \mathbb{T}^n; \ d^{\mathbb{T}^n}(x_0, x) < S_0/2\}$$
 (4.8)

Let  $H^h_{\Omega}$  be the selfadjoint operator on  $L^2(\Omega; \mathbb{C}^2)$  associated with  $P^h(x, hD)$  with Dirichlet boundary condition. We denote by  $(\lambda_j(H^h_{\Omega}))_{j\in\mathbb{N}^*}$  the increasing sequence of eigenvalues of  $H^h_{\Omega}$ . Using the method of [He-Sj-1], we get easily the following results

**Theorem 4.1** For any  $\eta$ ,  $0 < \eta < S_0/2$ , there exist  $h_0 > 0$  and  $N_0 > 1$  such that, if  $0 < h < h_0$  and  $j \le N_0$ , then

$$\forall \theta \in \mathbb{B}^n, \quad 0 < \lambda_j(H_{\Omega}^h) - \lambda_j^{h,\theta} \le C e^{-(S_0 - \eta)/(2h)}; \tag{4.9}$$

so the length of the band  $b_j^h$  satisfies  $|b_j^h| \leq Ce^{-(S_0 - \eta)/(2h)}$ .

For the first band, we have the following improvement

$$|b_1^h| \le Ce^{-(S_0 - \eta)/h}. (4.10)$$

Sketch of the proof.

As  $\Omega$  is simply connected and the one form  $\theta dx$  is closed, there exists a smooth real function  $\psi_{\theta}(x)$  on  $\overline{\Omega}$  such that  $e^{-i\psi_{\theta}(x)}P^h(x,hD)e^{i\psi_{\theta}(x)}=P^h(x,h(D-\theta))$ : the Dirichlet operators on  $\Omega$ ,  $H^h_{\Omega}$  and  $H^{h,\theta}_{\Omega}$  associated to  $P^h(x,hD)$  and  $P^h(x,h(D-\theta))$  are gauge equivalent, so they have the same spectrum.

Therefore the min-max principle says that

$$0 < \lambda_j(H_{\Omega}^{h,\theta}) - \lambda_j^{h,\theta} = \lambda_j(H_{\Omega}^h) - \lambda_j^{h,\theta}.$$

But the exponential decay of the eigenfunction  $\varphi_i^{h,\theta}(x)$  associated with  $\lambda_i^{h,\theta}$ , given by (4.7) implies that

$$\|(P^h(x, h(D-\theta)) - \lambda_i^{h,\theta})\chi\varphi_i^{h,\theta}(x)\|_{L^2(\Omega;\mathbb{C}^2)} \le Ce^{-(S_0 - \eta + \epsilon)/(2h)}$$

for some  $\epsilon > 0$ , and for a smooth cut-off function  $\chi$  supported in  $\Omega$  and  $\chi(x) = 1$ if  $d^{\mathbb{T}^n}(x_0, x) \leq (S_0 - \eta + \epsilon)/2$ . So  $distance(\lambda_j^{h,\theta}, \operatorname{sp}(H_{\Omega}^h)) \leq Ce^{-(S_0 - \eta + \epsilon)/(2h)}$ .

This achieves the proof of (4.9).

Let us denote  $E^{h,\theta}$ , (respectively  $E^{h,\Omega}$ ), the first eigenvalue  $\lambda_1^{h,\theta}$ , (respectively  $\lambda_1(H_{\Omega}^h)$ ), and  $\varphi^{h,\theta}(x)$ , (respectively  $\varphi^{h,\Omega}(x)$ ), the associated normalized eigenfunctions. Let  $\chi$  be a cut-off function satisfying the same properties as before. Then  $P^{h}(x, h(D-\theta))(e^{-i\psi_{\theta}(x)}\chi(x)\varphi^{h,\Omega}(x)) = \lambda_{1}(H_{\Omega}^{h})e^{-i\psi_{\theta}(x)}\chi(x)\varphi^{h,\Omega}(x) + e^{-i\psi_{\theta}(x)}r_{0}^{h}(x)$ with, thanks to the same identity as (4.7) for Dirichlet problem on  $\Omega$ ,

$$||r_0^h||_{L^2(\mathbb{T}^n;\mathbb{C}^2)} \le Ce^{-\frac{S_0-\eta}{2h}}.$$

The same argument used in [He-Sj-1], (see also [He]), gives this estimate

$$|E^{h,\theta} - E^{h,\Omega} - \langle r_0^h | \chi \varphi^{h,\Omega} \rangle_{L^2(\mathbb{T}^n:\mathbb{C}^2)} | \leq C e^{-(S_0 - \eta)/h}.$$

As  $\tau_h = \langle r_0^h | \chi \varphi^{h,\Omega} \rangle_{L^2(\mathbb{T}^n;\mathbb{C}^2)}$  does not depend on  $\theta$ , so

$$\forall \theta \in \mathbb{B}^n$$
,  $|E^{h,\theta} - E^{h,\Omega} - \tau_h| \le Ce^{-(S_0 - \eta)/h}$ 

this estimate ends the proof of (4.10)

As for the tunnel effect in [He-Sj-1] and [Si-2], we have an accuracy estimate for the first band, like the scalar case in [Si-3] and in [Ou] (see also [He]).

**Theorem 4.2** There exists  $h_0 > 0$  such that, if  $0 < h < h_0$  then

$$|b_1^h| \le Ce^{-S_0/h}.$$

Sketch of the proof. Instead of comparing  $H^{h,\theta}$  with an operator defined in a subset of  $\mathbb{T}^n$ , we have to work on the universal cover  $\mathbb{R}^n$  of  $\mathbb{T}^n$ .

We take  $\Omega \subset \mathbb{R}^n$  an open and simply connected set with smooth boundary satisfying, for some  $\eta_0$ ,  $0 < \eta_0 < \eta_1 < S_0/2$ ,

$$B_0((S_0 + \eta_0)/2) \subset \Omega \subset B_0((S_0 + \eta_1)/2).$$
 (4.11)

So  $\Omega$  contains the Wigner set  $\mathbb{W}^n$ , more precisely

$$\mathbb{W}^n \subset \Omega \subset 2\mathbb{W}^n \text{ and } \Omega \cap \Gamma = \{0\}.$$

We let also denote  $H^h_{\Omega}$  the Dirichlet operator on  $L^2(\Omega; \mathbb{C}^2)$  associated with  $P^h(x,hD)$ , and  $E^h_{\Omega}$  its first eigenvalue. The associated eigenfunction is also denoted by  $\varphi^{h,\Omega}(x)$ .

In the same way as to get (4.7), we have

$$\sum_{k=1}^{n} h^{2} \| (D_{x_{k}}I - A_{k})e^{d_{0}(x)/h} \varphi^{h,\Omega} \|_{L^{2}(\Omega;\mathbb{C}^{2})}^{2} \le hC \int_{B_{0}(\sqrt{h}C)} |\varphi^{h,\Omega}(x)|^{2} dx, \qquad (4.12)$$

then the Poincaré estimate gives

$$\int_{\Omega} e^{2d_0(x)/h} |\varphi^{h,\Omega}(x)|^2 dx \le h^{-1} C \int_{B_0(\sqrt{h}C)} |\varphi^{h,\Omega}(x)|^2 dx. \tag{4.13}$$

Let  $\chi$  a smooth cut-off function satisfying

$$\chi(x) = 1 \text{ if } d_0(x) \le (S_0 + \eta_0)/2 \text{ and } \chi(x) = 0 \text{ if } x \notin \Omega.$$

Then the function

$$\varphi^{h,\theta}(x) \, = \, \sum_{\omega \in \Gamma} e^{i\theta(x-\omega)} \chi(x-\omega) \varphi^{h,\Omega}(x-\omega)$$

is  $\Gamma$ -periodic and satisfies

$$\left(P^{h}(x, h(D-\theta)) - E_{\Omega}^{h}\right) \varphi^{h,\theta}(x) = r^{h,\theta} \text{ and} 
\|r^{h,\theta}\|_{L^{2}(\mathbb{W}^{n};\mathbb{C}^{2})} \leq Ce^{-(S_{0}+\eta_{0})/(2h)} \|\varphi^{h,\theta}\|_{L^{2}(\mathbb{W}^{n};\mathbb{C}^{2})} \right\}$$
(4.14)

and 
$$\langle r^{h,\theta} | \varphi^{h,\theta} \rangle_{L^2(\mathbb{W}^n;\mathbb{C}^2)} =$$

$$\sum_{\omega,\rho\in\Gamma_0} e^{i\theta(\rho-\omega)} \int_{\mathbb{W}^n} ([P^h(x,hD);\chi]\varphi^{h,\Omega})(x-\omega).\overline{(\chi\varphi^{h,\Omega})}(x-\rho)dx$$

with  $\Gamma_0 = \{0, \pm \beta_1, \dots, \pm \beta_n\}$  and

$$[P^{h}(x, hD); \chi] = -2h^{2}i \sum_{k=1}^{n} \partial_{x_{k}} \chi(D_{x_{k}}I - A_{k}) - h^{2}\Delta \chi I.$$

So

$$\left| \frac{1}{\|\varphi^{h,\theta}\|_{L^{2}(\mathbb{W}^{n}:\mathbb{C}^{2})}^{2}} < r^{h,\theta} \,|\, \varphi^{h,\theta} >_{L^{2}(\mathbb{W}^{n};\mathbb{C}^{2})} \right| \leq Ce^{-S_{0}/h}. \tag{4.15}$$

The proof comes easily from (4.12) and (4.13) as in [Ou] or in [He].

Using the same argument of [He-Sj-1] as in the proof of (4.10), we get that

$$|E^{h,\theta} - E^h_{\Omega} - \tau^{h,\theta}| \le Ce^{-(S_0 + \eta_0)/h}),$$
 (4.16)

with 
$$\tau^{h,\theta} = \frac{1}{\|\varphi^{h,\theta}\|_{L^2(\mathbb{W}^n;\mathbb{C}^2)}^2} < r^{h,\theta} | \varphi^{h,\theta} >_{L^2(\mathbb{W}^n;\mathbb{C}^2)}.$$

Theorem 4.2 follows from (4.15) and (4.16)

## 5 B.K.W. method for the Dirichlet ground state

Let  $\Omega$  be an open set satisfying (4.8). more precisely  $\Omega \subset \mathbb{R}^n$  an open, bounded and simply connected set with smooth boundary satisfying, for some  $\eta_1$  and  $\eta_2$ ,  $0 < \eta_1 < \eta_2 < S_0/2$ ,

$$\{x \in \mathbb{R}^n; \ d_0(x) < \frac{S_0 - \eta_2}{2}\} \subset \Omega \subset \{x \in \mathbb{R}^n; \ d_0(x) < \frac{S_0 - \eta_1}{2}\}$$
 (5.1)

**Theorem 5.1** The first eigenvalue  $E^{h,\Omega} = \lambda_1(H_{\Omega}^h)$  of the Dirichlet operator  $H_{\Omega}^h$  admits an asymptotic expansion of the form

$$E^{h,\Omega} \simeq \sum_{j=0}^{\infty} h^j e_j$$
,

and if  $S_0 - \eta_1$  is small enough, the associated eigenfunction  $\varphi^{h,\Omega}$  has also an asymptotic expansion of the form

$$\varphi^{h,\Omega} = e^{-\phi/h}(f_h^+, f_h^-) , \quad f_h^{\pm} \simeq \sum_{j=0}^{\infty} h^j f_j^{\pm} , \quad (f_0^- = 0) .$$

As usual

$$e_0 = E_0, \quad e_1 = \tau_1, \quad e_2 = r_{11}(0) + \sum_{k=1}^n |a_{k,11}(0)|^2,$$
 (5.2)

and  $\phi$  is the real function satisfying the eikonal equation

$$|\nabla \phi(x)|^2 = v(x) - |w(x)| - E_0,$$
 (5.3)

equal to d(x) in a neighbourhood of 0.

( $r_{11}$  and the  $a_{k,11}$  are defined by (1.1) and (1.3).  $E_0$  and  $\tau_1$  are defined by (2.2) and (2.4)).

*Proof.* When the gauge potential matrix is identified with the one form

$$Adx = \sum_{k=1}^{n} A_k(x) dx_k \,,$$

its curvature form appears to be the related magnetic field  $B = dA + A \wedge A$ :

$$B = \sum_{1 \leq j < k \leq n} (\partial_{x_j} A_k(x) - \partial_{x_k} A_j(x)) dx_j \wedge dx_k + \sum_{1 \leq j < k \leq n} (A_j(x) A_k(x) - A_k(x) A_j(x)) dx_j \wedge dx_k.$$

For our purpose, only the vector magnetic potential  $a_{.,11}$  is significant. We will work with Coulomb vector gauge  $a_{.,11}$ :

$$div(a_{.,11}(x)) = \sum_{k=1}^{n} \partial_{x_k} a_{k,11}(x) = 0.$$
 (5.4)

It is feasible thanks to the existence of a smooth real and  $\Gamma$  periodic function  $\psi(x)$  such that  $\Delta \psi(x) = div(a_{.,11}(x))$ .

Let  $\mathcal{O}$  be any open set of  $\mathbb{R}^n$  (or one can take also  $\mathcal{O} = \mathbb{T}^n$ ). Conjugation of  $P^h(x, hD)$  by the unitary operator  $J_{\psi}$  on  $L^2(\mathcal{O}; \mathbb{C}^2)$ :

$$J_{\psi} = \begin{pmatrix} e^{i\psi} & 0\\ 0 & e^{-i\psi} \end{pmatrix}, \tag{5.5}$$

leads to changing  $a_{.,11}(x)$  for  $a_{.,11}(x) - \nabla \psi(x)$  and  $a_{.,21}(x)$  for  $e^{2i\psi(x)}a_{.,21}(x)$ ; the new  $a_{.,22}(x)$  is equal to minus the new  $a_{.,11}(x)$ , and the new  $a_{.,12}(x)$  remains the conjugate of the new  $a_{.,21}(x)$ . So by (2.8) we have

$$\begin{aligned} a_{.,11} &= \beta \nabla \alpha - \alpha \nabla \beta + \delta \nabla \rho - \rho \nabla \delta - \nabla \psi \,, \\ a_{.,21} &= e^{2i\psi} [(\rho \nabla \beta - \beta \nabla \rho + \delta \nabla \alpha - \alpha \nabla \delta) + i(\alpha \nabla \rho - \rho \nabla \alpha + \delta \nabla \beta - \beta \nabla \delta)] \\ a_{.,22} &= -a_{.,11} \,, \quad a_{.,12} &= \overline{a_{.,21}} \\ \Delta \psi &= div (\beta \nabla \alpha - \alpha \nabla \beta + \delta \nabla \rho - \rho \nabla \delta) \end{aligned}$$

Let us write

$$e^{-\phi/h}P^h(x,hD)(e^{-\phi/h}f_h) = W_0(x)f_h + hW_1(x,D)f_h + h^2W_2(x,D)f_h$$
 (5.7)

with

$$W_0(x) = V(x) - |\nabla \phi(x)|^2 I$$

$$W_1(x, D) = \Delta \phi I + 2i \sum_{k=1}^n \partial_{x_k} \phi(D_{x_k} I - A_k)$$

$$W_2(x, D) = \sum_{k=1}^n (D_{x_k} I - A_k)^2 + R(x).$$

So

$$W_1(x,D) = \begin{pmatrix} \Delta \phi - 2i \nabla \phi. (i \nabla + a_{.,11}) & -2i \nabla \phi. \overline{a_{.,21}} \\ -2i \nabla \phi. a_{.,21} & \Delta \phi - 2i \nabla \phi. (i \nabla - a_{.,11}) \end{pmatrix},$$

and

$$W_2(x,D) = \begin{pmatrix} (i\nabla + a_{.,11})^2 + r_{11} & (i\nabla + a_{.,11}).\overline{a_{.,21}} + \overline{a_{.,21}}.(i\nabla - a_{.,11}) + r_{12} \\ a_{.,21}.(i\nabla + a_{.,11}) + (i\nabla + a_{.,11}).a_{.,21} + r_{21} & (i\nabla - a_{.,11})^2 + r_{22} \end{pmatrix}$$

We look for an eigenvalue  $E^h \simeq \sum_{j=0}^{\infty} h^j e_j$ 

and an associated eigenfunction  $f_h \simeq \sum_{j=0}^{\infty} h^j f_j$ , so

$$e^{\phi/h}(P^h(x,hD) - E^hI)(e^{-\phi/h}f_h) \simeq \sum_{j=0}^{\infty} h^j \kappa_j$$

with

$$\begin{split} \kappa_0(x) &= (W_0(x) - e_0 I) f_0(x) \\ \kappa_1(x) &= (W_1(x,D) - e_1 I) f_0(x) + (W_0(x) - e_0 I) f_1(x) \\ \kappa_2(x) &= (W_2(x,D) - e_2 I) f_0(x) + (W_1(x,D) - e_1 I) f_1(x) + (W_0(x) - e_0 I) f_2(x) \\ \kappa_j(x) &= -e_j f_0(x) - \sum_{\ell=1}^{j-3} e_{j-\ell} f_\ell(x) + (W_2(x,D) - e_2 I) f_{j-2}(x) \\ &+ (W_1(x,D) - e_1 I) f_{j-1}(x) + (W_0(x) - e_0 I) f_j(x), \ (j>2). \end{split}$$

We recall that  $f_j = (f_j^+, f_j^-)$  and we want that  $\kappa_j(x) = 0$ ,  $\forall j$ .

## 1) Term of order 0

As 
$$\kappa_0(x) = 0 \Leftrightarrow \begin{cases} (-|\nabla \phi(x)|^2 + v(x) - |w(x)| - e_0) f_0^+(x) = 0 \\ (-|\nabla \phi(x)|^2 + v(x) + |w(x)| - e_0) f_0^-(x) = 0 \end{cases}$$

choosing  $\phi$  satisfying (5.3), then

$$e_0 = E_0$$
 and  $-|\nabla \phi(x)|^2 + v(x) + |w(x)| - e_0 = 2|w(x)| > 0$  implies that

$$f_0^-(x) = 0$$
,  $e_0 = E_0$  and  $W_0(x) - e_0 I = \begin{pmatrix} 0 & 0 \\ 0 & 2|w(x)| \end{pmatrix}$ . (5.8)

#### 2) Term of order 1.

The components of  $\kappa_1(x) = (\kappa_1^+(x), \kappa_1^-(x))$  become

$$\kappa_1^+(x) = (\Delta\phi(x) - e_1 - 2ia_{.,11}(x).\nabla\phi(x))f_0^+(x) + 2\nabla\phi(x).\nabla f_0^+(x)$$
  

$$\kappa_1^-(x) = 2|w(x)|f_1^-(x) - 2i(a_{.,21}(x).\nabla\phi(x))f_0^+(x),$$

As  $|\nabla \phi(x)|$  has a simple zero at  $x_0 = 0$ , the equation  $\kappa_1^+(x) = 0$  can be solved only when  $e_1 = \Delta \phi(0)$ . In this case there exists a unique function  $f_0^+(x)$  such that  $f_0^+(0) = 1$  and  $\kappa_1^+(x) = 0$ . We can conclude that the study of the term of order 1 leads to

$$\begin{cases}
e_1 = \Delta\phi(0), \\
2\nabla\phi(x).\nabla f_0^+(x) = [e_1 - \Delta\phi(x) + 2ia_{.,11}(x).\nabla\phi(x)]f_0^+(x), \\
f_1^-(x) = \frac{i}{|w(x)|}(\nabla\phi(x).a_{.,21}(x))f_0^+(x).
\end{cases} (5.9)$$

#### 3) Term of order 2.

The components of  $\kappa_2(x) = (\kappa_2^+(x), \kappa_2^-(x))$  become

$$\kappa_{2}^{+}(x) = ((i\nabla + a_{.,11})^{2} + +r_{11}(x) - e_{2})f_{0}^{+}(x) + (\Delta\phi(x) - e_{1} - 2ia_{.,11}(x).\nabla\phi(x))f_{1}^{+}(x) + 2\nabla\phi(x).\nabla f_{1}^{+}(x) - 2i(\overline{a_{.,21}(x)}.\nabla\phi(x))f_{1}^{-}(x) \kappa_{2}^{-}(x) = 2|w(x)|f_{2}^{-}(x) - 2i(a_{.,21}(x).\nabla\phi(x))f_{1}^{+}(x) + 2\nabla\phi(x).\nabla f_{1}^{-}(x) + 2ia_{.,11}(x).\nabla\phi(x)f_{1}^{-}(x) + 2ia_{.,21}(x).\nabla f_{0}^{+}(x) + i(div(a_{.,21}(x))f_{0}^{+}(x) + r_{21}(x)f_{0}^{+}(x),$$

$$(5.10)$$

The unknown function  $f_1^+(x)$  must give  $\kappa_2^+(x) = 0$  in (5.10). This equation, with the initial condition  $f_1^+(0) = 0$ , can be solved only if

$$e_2 = (i\nabla + a_{.,11})^2 f_0^+(0) + r_{11}(0).$$

(We used that  $f_0^+(0) = 1$ ). So  $\kappa_2 = 0$  implies

$$\begin{array}{l} e_2 = (i\nabla + a_{.,11})^2 f_0^+(0) + r_{11}(0)\,, \\ 2\nabla\phi(x).\nabla f_1^+(x) = -(\Delta\phi(x) - e_1 - 2ia_{.,11}(x).\nabla\phi(x))f_1^+(x) \\ -((i\nabla + a_{.,11})^2 + e_2 - r_{11}(x))f_0^+(x) + 2i(a_{.,12}(x).\nabla\phi(x))f_1^-(x) \\ f_2^-(x) = \frac{1}{2|w(x)|} [2i(a_{.,21}(x).\nabla\phi(x))f_1^+(x) - 2\nabla\phi(x).\nabla f_1^-(x) - 2i(a_{.,11}(x).\nabla\phi(x))f_1^-(x) \\ -2ia_{.,21}(x).\nabla f_0^+(x) - i(div(a_{.,21}(x))f_0^+(x) - r_{21}(x)f_0^+(x)] \,. \end{array}$$

### 4) Term of order j > 2.

We assume that  $e_{\ell}$  for  $\ell = 0, 1, \ldots, j-1$ , the functions  $f_{\ell}^{\pm}(x)$  for  $\ell = 0, 1, \ldots, j-2$ , and the one  $f_{j-1}^{-}(x)$  are well-known,  $f_{\ell}^{+}(0) = 0$  when  $0 < \ell < j-1$ .

The equation  $\kappa_i^+ = 0$  becomes

$$2\nabla\phi(x).\nabla f_{j-1}^{+}(x) + (\Delta\phi(x) - e_{1} - 2ia_{.,11}(x).\nabla\phi(x))f_{j-1}^{+}(x) = 2i(\overline{a_{.,21}(x)}.\nabla\phi(x))f_{j-1}^{-}(x) + \sum_{\ell=0}^{j-3}e_{j-\ell}f_{\ell}^{+}(x) \\
-((i\nabla + a_{.,11})^{2} - e_{2} + r_{11}(x))f_{j-2}^{+}(x) \\
-(r_{12}(x) + idiv(\overline{a_{21}}))f_{j-2}^{-}(x) - 2i\overline{a_{21}}.\nabla f_{j-2}^{-}(x)$$
(5.11)

This equation has a unique solution  $f_{j-1}^+(x)$  such that  $f_{j-1}^+(0)=0$  iff

$$\begin{cases}
e_j = ((i\nabla + a_{.,11})^2 + r_{11}(0))f_{j-2}^+(0) + r_{12}(0)f_{j-2}^-(0) \\
-2i\overline{a_{.,21}(0)}.\nabla)f_{j-2}^-(0) - \sum_{\ell=0}^{j-3} e_{j-\ell}f_{\ell}^+(0).
\end{cases}$$
(5.12)

The equation  $\kappa_j^- = 0$  gives

$$f_j^-(x) = \frac{1}{2|w(x)|} \times$$

$$[-2\nabla\phi(x).\nabla f_{j-1}^{-}(x) + (e_1 - 2ia_{.,11}(x).\nabla\phi(x))f_{j-1}^{-}(x) + 2ia_{.,21}(x).\nabla\phi(x)f_{j-1}^{+}(x) + (e_2 - (i\nabla - a_{.,11})^2)f_{j-2}^{-}(x) - idiv(a_{.,21}(x))f_{j-2}^{+}(x) - 2ia_{.,21}(x).\nabla f_{j-2}^{+}(x) + \sum_{\ell=0}^{j-3} e_{j-\ell}f_{\ell}^{-}(x)]$$

## 5) End of the proof.

Let  $\chi(x)$  be a cut-off function equal to 1 in a neighbourhood of 0 and supported in  $\Omega$ . Then taking  $\chi(x)f_j(x)$  instead of  $f_j(x)$ , we get a function  $\varphi^{h,\Omega}$  satisfying Dirichlet boundary condition and Theorem 5.1. The self-adjointness of the related operator ensures that the computed sequence  $(e_j)$  is real  $\square$ 

## 6 Sharp asymptotic for the width of the first band

Returning to the proof of Theorem 4.2, we have to study carefully the  $\tau^{h,\theta}$  defined in (4.16), using the method of [He-Sj-1] performed in [He] and [Ou].

Using (4.14)–(4.16), we have

$$\tau^{h,\theta} = \sum_{\omega \in \Gamma_0^+} \left( e^{-i\theta\omega} (\rho_\omega^+ + \rho_\omega^-) + e^{i\theta\omega} \overline{(\rho_\omega^+ + \rho_\omega^-)} \right) , \qquad (6.1)$$

with  $\Gamma_0^+ = \{\beta_1, \dots, \beta_n\}$ ,

$$\rho_{\omega}^{+} = \frac{1}{\|\varphi^{h,\theta}\|_{L^{2}(\mathbb{W}^{n};\mathbb{C}^{2})}^{2}} \int_{\mathbb{W}^{n}} ([P^{h}(x,hD);\chi]\varphi^{h,\Omega})(x-\omega).\overline{(\chi\varphi^{h,\Omega})}(x)dx$$

and 
$$\rho_{\omega}^- = \frac{1}{\|\varphi^{h,\theta}\|_{L^2(\mathbb{W}^n,\mathbb{C}^2)}^2} \int_{\mathbb{W}^n} ([P^h(x,hD);\chi]\varphi^{h,\Omega})(x).\overline{(\chi\varphi^{h,\Omega})}(x+\omega)dx$$
.

We get from the formula of  $[P^h(x, hD); \chi]$  and from the estimate (4.13) that

$$\rho_{\omega}^{+} = -\frac{h^{2}}{\|\varphi^{h,\theta}\|_{L^{2}(\mathbb{W}^{n};\mathbb{C}^{2})}^{2}} \int_{\mathbb{W}^{n}} (\nabla \chi(x-\omega) \nabla \varphi^{h,\Omega})(x-\omega) . \overline{(\chi\varphi^{h,\Omega})}(x) dx + (6.2)$$
$$+ \mathbf{O}(he^{-S_{0}/h})$$

and

$$\rho_{\omega}^{-} = -\frac{h^{2}}{\|\varphi^{h,\theta}\|_{L^{2}(\mathbb{W}^{n};\mathbb{C}^{2})}^{2}} \int_{\mathbb{W}^{n}} (\nabla \chi(x) \nabla \varphi^{h,\Omega})(x) . \overline{(\chi \varphi^{h,\Omega})}(x+\omega) dx + \mathbf{O}(he^{-S_{0}/h}).$$

**Theorem 6.1** Under the assumption of Theorem 4.2, if for any  $\omega \in \{\pm \beta_1, \ldots, \pm \beta_n\}$  such that the Agmon distance in  $\mathbb{R}^n$  between 0 and  $\omega$  is the least one, (i.e.  $d(0,\omega) = S_0$ ), there exists one or a finite number of minimal geodesics joining 0 and  $\omega$ , then there exists  $\eta_0 > 0$  and  $h_0 > 0$  such that

$$b_1^h = \eta_0 h^{1/2} e^{-S_0/h} \left( 1 + \mathbf{O}(h^{1/2}) \right), \quad \forall h \in ]0, h_0[.$$

Sketch of the proof. Following the proof of splitting in [He-Sj-1] and [He], in (6.2) we can change  $\mathbb{W}^n$  into  $\mathbb{W}^n \cap \mathcal{O}$ , where  $\mathcal{O}$  is any neighbourhood of the minimal geodesics between 0 and the  $\pm \beta_k$ , such that  $d(x) = d(0, x) \in C^{\infty}(\mathcal{O})$ . In this case the B.K.W. method is valid in  $\mathbb{W}^n \cap \mathcal{O}$ . If  $\varphi_{B.K.W.}^h$  is the B.K.W. approximation of  $\varphi^{h,\Omega}$  in  $\mathbb{W}^n \cap \mathcal{O}$ , then, thanks to (4.1), for any  $p_0 > 0$  there exists  $C_{p_0}$  such that

$$h \sum_{k=1}^{n} \| (D_{x_k} I - A_k) e^{d(x)/h} \chi_0(\varphi^{h,\Omega} - \varphi^h_{B.K.W.}) \|_{L^2(\mathbb{W}^n;\mathbb{C}^2)}^2$$

$$+ \| e^{d(x)/h} \chi_0(\varphi^{h,\Omega} - \varphi^h_{B.K.W.}) \|_{L^2(\mathbb{W}^n;\mathbb{C}^2)}^2 \leq h^{p_0} C_{p_0},$$
(6.3)

where  $\chi_0$  is a cut-off function supported in  $\mathbb{W}^n \cap \mathcal{O}$  and equal to 1 in a neighborhood of the minimal geodesics between 0 and the  $\pm \beta_k$ . We have assumed that  $\|\varphi^{h,\Omega}\|_{L^2(\mathbb{W}^n;\mathbb{C}^2)} = 1$  and then  $\|\chi_0\varphi^h_{B.K.W.})\|_{L^2(\mathbb{W}^n;\mathbb{C}^2)}^2 - 1 = \mathbf{O}(h^p)$  for any p > 0.

As (6.2) remains valid if we change  $\varphi^{h,\Omega}$  into  $\chi_0\varphi^{h,\Omega}$ , the estimate (6.3) allows also to change  $\varphi^{h,\Omega}$  into  $\chi_0\varphi^h_{B.K.W.}$ . As a consequence, Theorem 6.1 follows easily, if in  $\mathbb{W}^n \cap \mathcal{O}$ ,  $\chi(x) = \chi_1(d(x))$  for a decreasing function  $\chi_1$  on  $[0, +\infty[$  with compact support, equal to 1 in a neighborhood of 0. In this case (6.2) becomes

$$\rho_{\omega}^{+} = \frac{h^{(2-n)/2}}{(2\pi)^{1/2} \prod_{k=1}^{n} \tau_{k}^{1/2}} \times \tag{6.4}$$

$$\int_{\mathbb{W}^n \cap \mathcal{O}} \chi_1'(d(x-\omega))\chi_1(d(x)) |\nabla d(x-\omega)|^2 f_0^+(x-\omega) f_0^+(x) e^{-(d(x-\omega)+d(x))/h} dx + \mathbf{O}(he^{-S_0/h})$$
 and

$$\rho_{\omega}^{-} = \frac{h^{(2-n)/2}}{(2\pi)^{1/2} \prod_{k=1}^{n} \tau_{k}^{1/2}} \times$$

$$\int_{\mathbb{W}^n\cap\mathcal{O}}\chi_1'(d(x))\chi_1(d(x+\omega))|\nabla d(x)|^2f_0^+(x)f_0^+(x+\omega)e^{-(d(x)+d(x+\omega))/h}dx+\mathbf{O}(he^{-S_0/h}).$$
 We remind that for any  $y$  in a minimal geodesic joining 0 to  $\pm\beta_k$ , if  $y\neq 0$  and

We remind that for any y in a minimal geodesic joining 0 to  $\pm \beta_k$ , if  $y \neq 0$  and  $y \neq \pm \beta_k$ , then the function  $d(x) + d(x \mp \beta_k)$ , when it is restricted to any hypersurface orthogonal to the geodesic through y, has a non degenerate minimum  $S_0$  at  $y\square$ 

#### Acknowledgement

The authors are grateful to Bernard Helffer for many discussions.

## References

- [Ag] S. Agmon: Lectures in exponential decay of solutions of second-order elliptic equations. Princeton University Press, Math. Notes 29.
- [Ca-Yu] M. Cardona, P. Y. Yur: Fundamentals of Semiconductors Physics and Materials Properties. Springer, Berlin 2010.
- [Co] N. R. Cooper: Optical Flux Lattices for Ultracold Atomic Gases. Phys. Rev. Lett. 106, (2011), 175301.
- [Co-Da] N. R. Cooper, J. Dalibard: Optical flux lattices for two-photon dressed states. Europhysics Letters, 95 (6), (2011), 66004.
- [Da-al] J. Dalibard, F. Gerbier, G. Juzeliunas, P. Ohberg: Colloquium: Artificial gauge potentials for neutral atoms. Rev. Mod. Phys. 83 (4), (2011), p. 1523-1543.
- [Di-Sj] M. Dimassi, J. Sjöstrand: Spectral asymptotics in the semi-classical limit. Cambridge University Press, 1999.

- [Ea] M. S. P. Eastham: The spectral theory of periodic differential equations. Scottish Academic, London 1974.
- [He] B. Helffer: Semi-classical analysis for the Schrödinger operator and applications. Lecture Notes in Math. 1336, Springer, 1988.
- [He-Sj-1] B. Helffer, J. Sjöstrand: Multiple wells in the semi-classical limit. Comm. in P.D.E., 8 (4), (1984), p.337-408.
- [He-Sj-2] B. Helffer, J. Sjöstrand: Effet tunnel pour l'équation de Schrödinger avec champ magnétique. Ann. Scuola Norm. Sup. Pisa, 14 (4), (1987), p. 625-657.
- [Hi-Si] P. D. Hislop, I. M. Sigal: Introduction to spectral theory. With applications to Schrödinger operators. Applied Mathematical Sciences, 113. Springer-Verlag, 1996.
- [Ou] A. Outassourt: Comportement semi-classique pour l'opérateur de Schrödinger à potentiel périodique. J. of Functional Analysis 72, (1987), p. 65-93.
- [Re-Si] M. Reed, B. Simon: Methods of modern mathematical physics, Vol 4. Academic Press, New York 1972.
- [Ro] D. Robert: Autour de l'approximation semi-classique. Birkhauser, 1986.
- [Si-1] B. Simon: Semi-classical analysis of low lying eigenvalues, I. Ann. Inst. H. Poincaré, 38, (1983), p. 295-307.
- [Si-2] B. Simon: Semiclassical analysis of low lying eigenvalues, II. Annals of Math. 120, (1984), p. 89-118.
- [Si-3] B. Simon: Semiclassical analysis of low lying eigenvalues, III. Ann. Physics, 158 (2), (1984), p. 295-307.