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

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Abstract

We consider a Schrödinger operator with a Hermitian 2×2 matrix-valued potential which is lattice periodic and can be diagonalized smoothly on the whole 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.

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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 :

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

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

$$P^h(x, \xi) = \sum_{k=1}^n \{(\xi_k I - hA_k(x))^2 + ih^2 \partial_{x_k} A_k(x)\} + V(x) + hQ(x) + h^2 R(x), \quad (1.2)$$

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 Γ periodic:

$$\left. \begin{aligned} A_k &= (a_{k,ij}(x))_{1 \leq i,j \leq m}, & V &= (v_{ij}(x))_{1 \leq i,j \leq m}, \\ Q &= (q_{ij}(x))_{1 \leq i,j \leq m}, & R &= (r_{ij}(x))_{1 \leq i,j \leq m}, \\ a_{k,ij}, v_{ij}, q_{ij}, r_{ij} &\in C^\infty(\mathbb{R}^n; \mathbb{C}), \\ \overline{a_{k,ji}} &= a_{k,ij}, \overline{v_{ji}} = v_{ij}, \overline{q_{ji}} = q_{ij}, \overline{r_{ji}} = r_{ij} \\ a_{k,ij}(x - \gamma) &= a_{k,ij}(x), v_{ij}(x - \gamma) = v_{ij}(x), \\ q_{ij}(x - \gamma) &= q_{ij}(x) \text{ and } r_{ij}(x - \gamma) = r_{ij}(x) \quad \forall \gamma \in \Gamma; \end{aligned} \right\} \quad (1.3)$$

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

$\beta_1, \beta_2, \dots, \beta_n \in \mathbb{R}^n$ form a basis, $\det(\beta_1, \beta_2, \dots, \beta_n) \neq 0$.

We use the notation $D = (D_{x_1}, \dots, D_{x_n})$ where $D_{x_k} = -i\partial_{x_k}$, $k = 1 \dots n$, so $D^2 = -\Delta$ is the Laplacian operator on $L^2(\mathbb{R}^n)$.

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

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

The fundamental cell, the Wigner-Seitz cell,

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

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

$$\mathbb{B}^n = \left\{ \sum_{k=1}^n \theta_k \beta_k^*; \theta_k \in]-\frac{1}{2}, \frac{1}{2}[\right\} .$$

We will identify $L^2(\mathbb{T}^n; \mathbb{C}^m)$ with Γ 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 Γ periodic functions of $W^k_{loc}(\mathbb{R}^n; \mathbb{C}^m)$ provided with the norm of $W^k(\mathbb{W}^n; \mathbb{C}^m)$.

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

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

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

$$\text{sp}(H^{h,\theta}) = \{ \lambda_j^{h,\theta}; j \in \mathbb{N}^* \}, \quad \lambda_1^{h,\theta} \leq \lambda_2^{h,\theta} \leq \dots \leq \lambda_j^{h,\theta} \leq \lambda_{j+1}^{h,\theta} \leq \dots \quad (1.4)$$

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

(When $m = 1$ and $V = Q = R = A_k = 0$, $(\frac{1}{\sqrt{|\mathbb{T}^n|}} e^{i\omega \cdot x})_{\omega \in \Gamma^*}$ 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

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

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 .

2 Preliminary: the artificial gauge model

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

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

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

Let us remark that

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

In the sequel we will assume that

$$\left. \begin{array}{l} |w| > 0 \\ v(x) - |w(x)| \text{ has a unique non degenerate minimum on } \mathbb{T}^n. \end{array} \right\} \quad (2.3)$$

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

$$\left. \begin{array}{l} v(\gamma) - |w(\gamma)| < v(x) - |w(x)|, \quad \forall x \in \mathbb{R}^n \setminus \Gamma \text{ and } \forall \gamma \in \Gamma, \\ v(x) - |w(x)| = E_0 + \sum_{k=1}^n \tau_k^2 x_k^2 + \mathbf{O}(|x|^3), \text{ as } |x| \rightarrow 0, \end{array} \right\} \quad (2.4)$$

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

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

$$U^* V U = \tilde{V} = \begin{bmatrix} v - |w| & 0 \\ 0 & v + |w| \end{bmatrix}. \quad (2.5)$$

As $|w|$ never vanishes, $U = U(x)$ can be chosen smooth and Γ 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 $u_{11} = \frac{1}{2\sqrt{|w|(|w| - \operatorname{Re}((w_1 + iw_2)e^{-i\theta}))}}(w_3 - |w| + e^{i\theta}(w_1 - iw_2)),$

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

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

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

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

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

σ_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

$$\tilde{H}^h = U^* H^h U = h^2 D^2 I + U^* V U - 2ih^2 \sum_{k=1}^n [(U^* \partial_{x_k} U) D_{x_k} - h^2 U^* \partial_{x_k}^2 U]$$

which can be rewritten as

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

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

$$A_k = [(\partial_{x_k} \alpha, \partial_{x_k} \beta, \partial_{x_k} \rho) \wedge (\alpha, \beta, \rho) + (\delta \partial_{x_k} \alpha - \alpha \partial_{x_k} \delta, \delta \partial_{x_k} \beta - \beta \partial_{x_k} \delta, \delta \partial_{x_k} \rho - \rho \partial_{x_k} \delta)] \cdot \sigma, \quad (2.8)$$

and

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

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 $V = \tilde{V}$ a diagonal matrix given by (2.5).

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

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

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

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

with

$$\left. \begin{aligned} P_{11}^h(x, hD) &= h^2(D - a_{.,11}(x))^2 + v(x) - |w(x)| + h^2 r_{11}(x) \\ P_{22}^h(x, hD) &= h^2(D + a_{.,11}(x))^2 + v(x) + |w(x)| + h^2 r_{22}(x) \\ P_{12}^h(x, hD) &= -h^2 a_{.,12}(x) \cdot (D + a_{.,11}(x)) - h^2 a_{.,12}(x) \cdot (D - a_{.,11}(x)) \\ &\quad + ih^2 \text{div}(a_{.,12}(x)) + h^2 r_{12}(x) \\ P_{21}^h(x, hD) &= -h^2 a_{.,21}(x) \cdot (D - a_{.,11}(x)) - h^2 a_{.,21}(x) \cdot (D + a_{.,11}(x)) \\ &\quad + ih^2 \text{div}(a_{.,21}(x)) + h^2 r_{21}(x). \end{aligned} \right\} \quad (3.2)$$

($D = (D_{x_1}, D_{x_2}, \dots, D_{x_n})$ 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 $c_1 = \max \|R(x)\|$,

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

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*

$$\left. \begin{aligned} E^h \in \text{sp}(H_{11}^{h,\theta}) &\Rightarrow \text{distance}(E^h, \text{sp}(H_{11}^{h,\theta})) \leq C_0 h^2 \\ E^h \in \text{sp}(H_{11}^{h,\theta}) &\Rightarrow \text{distance}(E^h, \text{sp}(H_{22}^{h,\theta})) \leq C_0 h^2. \end{aligned} \right\} \quad (3.3)$$

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 $\|(H_{22}^{h,\theta} - E^h)^{-1}\|_{L^2(\mathbb{T}^n)} + \|h(D - \theta)(H_{22}^{h,\theta} - E^h)^{-1}\|_{L^2(\mathbb{T}^n)} + \|(H_{22}^{h,\theta} - E^h)^{-1}h(D - \theta)\|_{L^2(\mathbb{T}^n)} + \|h(D - \theta)(H_{22}^{h,\theta} - E^h)^{-1}h(D - \theta)\|_{L^2(\mathbb{T}^n)} \leq C$, and then

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

So if $E^h \in \text{sp}(H_{11}^{h,\theta})$, then $u^h = (u_1^h, u_2^h) \neq (0, 0)$ is an eigenfunction of $H^{h,\theta}$ associated with E^h iff

$$\left. \begin{aligned} H_{11}^{h,\theta} u_1^h + P_{12}^h(x, h(D - \theta))u_2^h &= E^h u_1^h \\ u_2^h &= -(H_{22}^{h,\theta} - E^h)^{-1}P_{21}^h(x, h(D - \theta))u_1^h. \end{aligned} \right\} \quad (3.4)$$

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

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

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 $\forall j \leq N_0, |\lambda_j(H_{11}^{h,\theta}) - (h\mu_j^h + E_0)| \leq C_0 h^2 \square$

4 Asymptotic of the first band

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

$$\left. \begin{aligned} \operatorname{Re} \left(\langle P^h(x, h(D - \theta))u \mid e^{2\phi/h}u \rangle_{L^2(\mathbb{T}^n; \mathbb{C}^2)} \right) = \\ \sum_{k=1}^n h^2 \| ((D_{x_k} - \theta_k)I - A_k)e^{\phi/h}u \|_{L^2(\mathbb{T}^n; \mathbb{C}^2)}^2 \\ + \langle (\tilde{V} - |\nabla\phi|^2 I + h^2 R)u \mid e^{2\phi/h}u \rangle_{L^2(\mathbb{T}^n; \mathbb{C}^2)} . \end{aligned} \right\} \quad (4.1)$$

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

$$d(y, x) = \inf_{\gamma} \int_0^1 \sqrt{v(\gamma(t)) - |w(\gamma(t))| - E_0} |\dot{\gamma}(t)| dt , \quad (4.2)$$

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 $|\nabla_x d(y, x)|^2 \leq v(x) - |w(x)| - E_0$ almost everywhere on \mathbb{R}^n .

Using that the zeros of $v(x) - w(x) - E_0$ are the elements of Γ 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:

$$\left. \begin{aligned} i) \quad & \exists R_0 > 0 \text{ s.t. } d_0(x) \in C^\infty(B_0(R_0)) \\ ii) \quad & |\nabla d_0(x)|^2 = v(x) - |w(x)| - E_0, \quad \forall x \in B_0(R_0) \\ iii) \quad & |\nabla d_0(x)|^2 \leq v(x) - |w(x)| - E_0 \\ iv) \quad & |\nabla d_\Gamma(x)|^2 \leq v(x) - |w(x)| - E_0 \end{aligned} \right\} \quad (4.3)$$

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 Γ is

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

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

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

Then

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

where x_0 is the single point in \mathbb{T}^n such that $v(x_0) - |w(x_0)| = E_0$. The Γ -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],

$$\left. \begin{aligned} & \sum_{k=1}^n h^2 \|((D_{x_k} - \theta_k)I - A_k)e^{\phi/h}u^{h,\theta}\|_{L^2(\mathbb{T}^n; \mathbb{C}^2)}^2 \\ & + \langle [\tilde{V} - |\nabla\phi|^2I + h^2R - \lambda^{h,\theta}I]_+ u^{h,\theta} | e^{2\phi/h}u^{h,\theta} \rangle_{L^2(\mathbb{T}^n; \mathbb{C}^2)} \\ & = \langle [\tilde{V} - |\nabla\phi|^2I + h^2R - \lambda^{h,\theta}I]_- u^{h,\theta} | e^{2\phi/h}u^{h,\theta} \rangle_{L^2(\mathbb{T}^n; \mathbb{C}^2)}, \end{aligned} \right\} \quad (4.6)$$

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

$$\left. \begin{aligned} & \sum_{k=1}^n h^2 \|((D_{x_k} - \theta_k)I - A_k)e^{\eta d^{\mathbb{T}^n}(x_0, x)/h}u^{h,\theta}\|_{L^2(\mathbb{T}^n; \mathbb{C}^2)}^2 \\ & + (1 - \eta^2) \langle (v - |w| - E_0)u^{h,\theta} | e^{2\eta d^{\mathbb{T}^n}(x_0, x)/h}u^{h,\theta} \rangle_{L^2(\mathbb{T}^n; \mathbb{C}^2)} \\ & \leq hC_\eta \int_{\{x \in \mathbb{T}^n; d^{\mathbb{T}^n}(x_0, x) < \sqrt{h}C\}} |u^{h,\theta}(x)|^2 dx. \end{aligned} \right\} \quad (4.7)$$

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

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

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

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

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

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

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

Sketch of the proof.

As Ω is simply connected and the one form θdx 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 Ω , H_Ω^h and $H_\Omega^{h,\theta}$ 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 $\varphi_j^{h,\theta}(x)$ associated with $\lambda_j^{h,\theta}$, given by (4.7) implies that

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

for some $\epsilon > 0$, and for a smooth cut-off function χ supported in Ω and $\chi(x) = 1$ if $d^{\mathbb{T}^n}(x_0, x) \leq (S_0 - \eta + \epsilon)/2$.

So $\text{distance}(\lambda_j^{h,\theta}, \text{sp}(H_\Omega^h)) \leq Ce^{-(S_0 - \eta + \epsilon)/(2h)}$.

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 χ 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 Ω ,

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

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

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

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

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

this estimate ends the proof of (4.10) \square

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*

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

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 η_0 , $0 < \eta_0 < \eta_1 < S_0/2$,

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

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

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

We let also denote H_Ω^h the Dirichlet operator on $L^2(\Omega; \mathbb{C}^2)$ associated with $P^h(x, hD)$, and E_Ω^h 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

$$\sum_{k=1}^n h^2 \|(D_{x_k} I - A_k) e^{d_0(x)/h} \varphi^{h, \Omega}\|_{L^2(\Omega; \mathbb{C}^2)}^2 \leq hC \int_{B_0(\sqrt{h}C)} |\varphi^{h, \Omega}(x)|^2 dx, \quad (4.12)$$

then the Poincaré estimate gives

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

Let χ a smooth cut-off function satisfying

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

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 Γ -periodic and satisfies

$$\left. \begin{aligned} (P^h(x, h(D-\theta)) - E_\Omega^h) \varphi^{h, \theta}(x) &= r^{h, \theta} \text{ and} \\ \|r^{h, \theta}\|_{L^2(\mathbb{W}^n; \mathbb{C}^2)} &\leq C e^{-(S_0 + \eta_0)/(2h)} \|\varphi^{h, \theta}\|_{L^2(\mathbb{W}^n; \mathbb{C}^2)} \end{aligned} \right\} \quad (4.14)$$

and

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

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

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

$$\left| \frac{1}{\|\varphi^{h, \theta}\|_{L^2(\mathbb{W}^n; \mathbb{C}^2)}^2} \langle r^{h, \theta} | \varphi^{h, \theta} \rangle_{L^2(\mathbb{W}^n; \mathbb{C}^2)} \right| \leq C e^{-S_0/h}. \quad (4.15)$$

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

$$|E^{h, \theta} - E_\Omega^h - \tau^{h, \theta}| \leq C e^{-(S_0 + \eta_0)/h}, \quad (4.16)$$

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

Theorem 4.2 follows from (4.15) and (4.16) \square

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

Let Ω 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 η_1 and η_2 , $0 < \eta_1 < \eta_2 < S_0/2$,

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

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

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

and ϕ is the real function satisfying the eikonal equation

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

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 τ_1 are defined by (2.2) and (2.4)).

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

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

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 $a_{.,11}$:

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

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

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_ψ on $L^2(\mathcal{O}; \mathbb{C}^2)$:

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

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

$$\left. \begin{aligned} a_{\cdot,11} &= \beta\nabla\alpha - \alpha\nabla\beta + \delta\nabla\rho - \rho\nabla\delta - \nabla\psi, \\ a_{\cdot,21} &= e^{2i\psi}[(\rho\nabla\beta - \beta\nabla\rho + \delta\nabla\alpha - \alpha\nabla\delta) + i(\alpha\nabla\rho - \rho\nabla\alpha + \delta\nabla\beta - \beta\nabla\delta)] \\ a_{\cdot,22} &= -a_{\cdot,11}, \quad a_{\cdot,12} = \overline{a_{\cdot,21}} \\ \Delta\psi &= \text{div}(\beta\nabla\alpha - \alpha\nabla\beta + \delta\nabla\rho - \rho\nabla\delta) \end{aligned} \right\} \quad (5.6)$$

Let us write

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

with

$$\begin{aligned} W_0(x) &= V(x) - |\nabla\phi(x)|^2 I \\ W_1(x, D) &= \Delta\phi I + 2i \sum_{k=1}^n \partial_{x_k} \phi (D_{x_k} I - A_k) \\ W_2(x, D) &= \sum_{k=1}^n (D_{x_k} I - A_k)^2 + R(x). \end{aligned}$$

So

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

and

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

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

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

with

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

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

1) Term of order 0

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

choosing ϕ satisfying (5.3), then

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

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

2) Term of order 1.

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

$$\begin{aligned}
\kappa_1^+(x) &= (\Delta\phi(x) - e_1 - 2ia_{.,11}(x) \cdot \nabla\phi(x)) f_0^+(x) + 2\nabla\phi(x) \cdot \nabla f_0^+(x) \\
\kappa_1^-(x) &= 2|w(x)| f_1^-(x) - 2i(a_{.,21}(x) \cdot \nabla\phi(x)) f_0^+(x),
\end{aligned}$$

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

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

3) Term of order 2.

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

$$\left. \begin{aligned} \kappa_2^+(x) &= ((i\nabla + a_{.,11})^2 + r_{11}(x) - e_2) f_0^+(x) \\ &\quad + (\Delta\phi(x) - e_1 - 2ia_{.,11}(x) \cdot \nabla\phi(x)) f_1^+(x) + 2\nabla\phi(x) \cdot \nabla f_1^+(x) \\ &\quad - 2i(a_{.,21}(x) \cdot \nabla\phi(x)) f_1^-(x) \\ \kappa_2^-(x) &= 2|w(x)| f_2^-(x) - 2i(a_{.,21}(x) \cdot \nabla\phi(x)) f_1^+(x) \\ &\quad + 2\nabla\phi(x) \cdot \nabla f_1^-(x) + 2ia_{.,11}(x) \cdot \nabla\phi(x) f_1^-(x) + 2ia_{.,21}(x) \cdot \nabla f_0^+(x) \\ &\quad + i(\text{div}(a_{.,21}(x))) f_0^+(x) + r_{21}(x) f_0^+(x), \end{aligned} \right\} \quad (5.10)$$

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

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

4) Term of order $j > 2$.

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

The equation $\kappa_j^+ = 0$ becomes

$$\left. \begin{aligned} 2\nabla\phi(x) \cdot \nabla f_{j-1}^+(x) + (\Delta\phi(x) - e_1 - 2ia_{\cdot,11}(x) \cdot \nabla\phi(x)) f_{j-1}^+(x) &= \\ 2i(\overline{a_{\cdot,21}(x)} \cdot \nabla\phi(x)) f_{j-1}^-(x) + \sum_{\ell=0}^{j-3} e_{j-\ell} f_\ell^+(x) & \\ -((i\nabla + a_{\cdot,11})^2 - e_2 + r_{11}(x)) f_{j-2}^+(x) & \\ -(r_{12}(x) + i\operatorname{div}(\overline{a_{21}})) f_{j-2}^-(x) - 2i\overline{a_{21}} \cdot \nabla f_{j-2}^-(x) & \end{aligned} \right\} \quad (5.11)$$

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

$$\left. \begin{aligned} e_j &= ((i\nabla + a_{\cdot,11})^2 + r_{11}(0)) f_{j-2}^+(0) + r_{12}(0) f_{j-2}^-(0) \\ &\quad - 2ia_{\cdot,21}(0) \cdot \nabla f_{j-2}^-(0) - \sum_{\ell=0}^{j-3} e_{j-\ell} f_\ell^+(0). \end{aligned} \right\} \quad (5.12)$$

The equation $\kappa_j^- = 0$ gives

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

$$\begin{aligned} &[-2\nabla\phi(x) \cdot \nabla f_{j-1}^-(x) + (e_1 - 2ia_{\cdot,11}(x) \cdot \nabla\phi(x)) f_{j-1}^-(x) + 2ia_{\cdot,21}(x) \cdot \nabla\phi(x) f_{j-1}^+(x) \\ &+ (e_2 - (i\nabla - a_{\cdot,11})^2) f_{j-2}^-(x) - i\operatorname{div}(a_{\cdot,21}(x)) f_{j-2}^+(x) - 2ia_{\cdot,21}(x) \cdot \nabla f_{j-2}^+(x) + \sum_{\ell=0}^{j-3} e_{j-\ell} f_\ell^-(x)] \end{aligned}$$

5) End of the proof.

Let $\chi(x)$ be a cut-off function equal to 1 in a neighbourhood of 0 and supported in Ω . 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

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

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

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

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

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

$$\begin{aligned} \rho_\omega^+ = & -\frac{h^2}{\|\varphi^{h,\theta}\|_{L^2(\mathbb{W}^n; \mathbb{C}^2)}^2} \int_{\mathbb{W}^n} (\nabla \chi(x - \omega) \nabla \varphi^{h,\Omega})(x - \omega) \cdot \overline{(\chi \varphi^{h,\Omega})}(x) dx + \\ & + \mathbf{O}(he^{-S_0/h}) \end{aligned} \quad (6.2)$$

and

$$\rho_\omega^- = -\frac{h^2}{\|\varphi^{h,\theta}\|_{L^2(\mathbb{W}^n; \mathbb{C}^2)}^2} \int_{\mathbb{W}^n} (\nabla \chi(x) \nabla \varphi^{h,\Omega})(x) \cdot \overline{(\chi \varphi^{h,\Omega})}(x + \omega) dx + \mathbf{O}(he^{-S_0/h}).$$

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

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

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

$$\begin{aligned} h \sum_{k=1}^n \|(D_{x_k} I - A_k) e^{d(x)/h} \chi_0 (\varphi^{h,\Omega} - \varphi_{B.K.W.}^h)\|_{L^2(\mathbb{W}^n; \mathbb{C}^2)}^2 \\ + \|e^{d(x)/h} \chi_0 (\varphi^{h,\Omega} - \varphi_{B.K.W.}^h)\|_{L^2(\mathbb{W}^n; \mathbb{C}^2)}^2 \leq h^{p_0} C_{p_0}, \end{aligned} \quad (6.3)$$

where χ_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 $\|\chi_0 \varphi_{B.K.W.}^h\|_{L^2(\mathbb{W}^n; \mathbb{C}^2)}^2 - 1 = \mathbf{O}(h^p)$ 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 $\chi_0\varphi_{B.K.W.}^h$. 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 χ_1 on $[0, +\infty[$ with compact support, equal to 1 in a neighborhood of 0. In this case (6.2) becomes

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

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

and

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

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

We remind that for any y in a minimal geodesic joining 0 to $\pm\beta_k$, if $y \neq 0$ and $y \neq \pm\beta_k$, 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

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