SÉMINAIRE DE THÉORIE SPECTRALE ET GÉOMÉTRIE

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Séminaire de Théorie spectrale et géométrie, tome 11 (1992-1993), p. 147-155

<http://www.numdam.org/item?id=TSG_1992-1993__11__147_0>

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GRENOBLE
1992–1993 (147–155)

SEMICLASSICAL EIGENSTATES IN A MULTIDIMENSIONAL WELL

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ABSTRACT. The two-dimensional Schrödinger operator with an analytic potential, having a non-degenerated minimum (well) at the origin, is considered. Under the Diophantine condition on the frequencies, the full asymptotic series (the Plank constant $\hbar$ tending to zero) for eigenfunctions with given quantum numbers (n_1, n_2), concentrated at the bottom of the well , is constructed, the Gaussian-like asymptotics being valid in a neighbourhood of the origin which is independent of $\hbar$. For small quantum numbers the second approximation to the eigenvalues is written in terms of the derivatives of the potential.

§1. INTRODUCTION

We consider the Schrödinger equation

$$-\frac{\hbar^2}{2}\Delta u + Vu = Eu \tag{1.1}$$

where $\Delta = \sum_{i=1}^{n} \frac{\partial^2}{\partial x_i^2}$ is the Laplace operator, V is a real valued function defined on $\mathbb{R}^n$. We are interested in the semiclassical ($\hbar \to 0$) asymptotics of the discrete spectrum of this operator in the case when the potential V has one or several nondegenerated minima, "wells".

If V has a finite number of identical wells which differ only by space translations, the spectrum of the corresponding Schrödinger operator is organized in the following way. There is a set of finite groups of eigenvalues, the distance between the groups being of the order $\hbar$, and the distance between eigenvalues in each group, the splitting, being exponentially small with respect to $\hbar$. The problem is to find the widths of these splittings. This problem was considered by different authors [1–8] and was completely solved in one-dymensional case. In multidimensional case the problem seems to be more difficult, and up to now there was no significant progress. In this paper, under some nondegeneracy conditions on V, we write down asymptotic series for eigenstates and the corresponding eigenvalues, the former being concentrated at the bottom of the well.

§2 ASYMPTOTIC EXPANSIONS FOR THE EIGENSTATES

For simplicity we consider the case of two dimensions but the case of n dimensions is in principle the same.

Let the potential V be analytic and represented by the the Taylor series

$$V(x_1, x_2) = \frac{\omega_1^2}{2}x_1^2 + \frac{\omega_2^2}{2}x_2^2 + \sum_{i+j\geq 3} v_{ij}x_1^i x_2^j \tag{2.1}$$

convergent in a bicylinder $|x_k| \leq r$, $k = 1, 2$, with $\omega_{1,2} > 0$.

We construct the asymptotic series for eigenvalues and eigenfunctions of (1.1) in the following form:

$$E_{n_1,n_2} = \sum_{k=1}^{\infty} E_k^{n_1,n_2} \hbar^k, \tag{2.2}$$

$$u_{n_1,n_2} = \sum_{\substack{0\leq i\leq 1,\\ 0\leq j\leq 1}} A_{ij}^{n_1,n_2} D_{n_1}^{(i)}\left(\frac{\psi_1}{\sqrt{\hbar}}\right) D_{n_2}^{(j)}\left(\frac{\psi_2}{\sqrt{\hbar}}\right) \hbar^{\frac{i+j}{2}}, \tag{2.3}$$

$$A_{ij}^{n_1,n_2} = \sum_{k=0}^{\infty} \left(A_{ij}^{n_1,n_2}\right)_k \hbar^k; \tag{2.4}$$

here $D_n^{(i)}$ denotes the i-th order derivative of the function of the parabolic cylinder i.e. the bounded solution of the Weber equation:

$$D''_{n_i}(t) = [t^2 - (2n_i + 1)]D_{n_i}(t), \quad D_n(t) = H_n e^{-\frac{t^2}{2}}, \quad H_n = \frac{e^{t^2}}{(-2)^n}\left(e^{-t^2}\right)^{(n)}, \tag{2.5}$$

$\psi_r = \psi_r(\vec{x})$, $\vec{x} = (x_1, x_2)$, $r = 1, 2$, $\left(A_{ij}^{n_1,n_2}\right)_k = \left(A_{ij}^{n_1,n_2}\right)_k(\vec{x})$, $k = 0, 1, 2, \ldots$ are functions independent of $\hbar$.

Substituting (2.2), (2.3) into (1.1) we find the following phase equation

$$(\nabla S)^2 = 2V, \tag{2.6}$$

for each of the phase functions

$$S^{\pm} = \frac{1}{2}\left(\psi_1^2 \pm \psi_2^2\right), \tag{2.7}$$

and the following recurrent systems for the amplitude coefficients $\left(A_{ij}^{n_1,n_2}\right)_k$ and numbers $E_k^{n_1,n_2}$

$$\mathbf{A}_0^{n_1,n_2}\vec{\mathcal{A}}_0 = 0, \tag{2.8}$$

$$\mathbf{A}_0^{n_1,n_2}\vec{\mathcal{A}}_k = -\sum_{r=1}^{k}\mathbf{A}_r^{n_1,n_2}\vec{\mathcal{A}}_{k-r}, \quad k=1,2,3,\ldots \tag{2.9}$$

where

$$\vec{\mathcal{A}}_k = \left((A_{00}^{n_1n_2})_k, (A_{10}^{n_1n_2})_k, (A_{01}^{n_1n_2})_k, (A_{11}^{n_1n_2})_k\right)^T = (\mathcal{A}_1^k, \mathcal{A}_2^k, \mathcal{A}_3^k, \mathcal{A}_4^k)^T,$$

T denoting transposition,

$$\mathbf{A}_0^{n_1,n_2} = \begin{pmatrix} -\varkappa & \hat{\mathbf{a}}_1 & \hat{\mathbf{a}}_2 & 0 \\ \mathbf{a}_1 & -\varkappa & 0 & \hat{\mathbf{a}}_2 \\ \mathbf{a}_2 & 0 & -\varkappa & \hat{\mathbf{a}}_1 \\ 0 & \mathbf{a}_2 & \mathbf{a}_1 & -\varkappa \end{pmatrix}, \tag{2.10}$$

$$\varkappa = \sum_{s=1}^{2}\frac{2n_s+1}{2}(\nabla\psi_s)^2 - E_1^{n_1n_2}, \tag{2.11}$$

$$\mathbf{a}_s = \nabla\psi_s \bullet \nabla + \frac{\Delta\psi_s}{2}, \tag{2.12}$$

the fat dot denoting a scalar product in $\mathbb{R}^n$,

$$\hat{\mathbf{a}}_s = \psi_s^2\left(\nabla\psi_s \bullet \nabla + \frac{\Delta\psi_s}{2}\right) + \psi_s(\nabla\psi_s)^2, \; s=1,2, \tag{2.13}$$

$$\mathbf{A}_1^{n_1n_2} = \begin{pmatrix} -\frac{1}{2}\Delta + E_2^{n_1n_2} & -\varkappa_1 & -\varkappa_2 & 0 \\ 0 & -\frac{1}{2}\Delta + E_2^{n_1n_2} & 0 & -\varkappa_2 \\ 0 & 0 & -\frac{1}{2}\Delta + E_2^{n_1n_2} & -\varkappa_1 \\ 0 & 0 & 0 & -\frac{1}{2}\Delta + E_2^{n_1n_2} \end{pmatrix}, \tag{2.14}$$

$$\varkappa_s = (2n_s+1)\nabla\psi_s \bullet \nabla + \frac{\Delta\psi_s}{2}, \quad s=1,2. \tag{2.15}$$

$$\mathbf{A}_k^{n_1n_2} = I_4 E_{k+1}^{n_1n_2}, \quad k=2,3,\ldots \tag{2.16}$$

I_4 denoting the 4×4 identity matrix.

In the next two sections we will describe shortly how the equations (2.6), (2.8), (2.9) can be solved.

§3 The phase functions.

In this section we consider the equation (2.6). We search solutions of the equation (2.6) in the form of the following power series

$$S^{\pm}(x_1,x_2)=\frac{\omega_1}{2}x_1^2\pm\frac{\omega_2}{2}x_2^2+\sum_{i+j\geq 3}S^{\pm}_{ij}x_1^ix_2^j \tag{3.1}$$

and find the recurrent formulae for the coeffitients

$$S^{\pm}_{ij}=\frac{\tilde{v}_{ij}}{i\omega_1\pm j\omega_2}, \tag{3.2}$$

where $\tilde{v}_{ij}$ depend on v_{ij} and $S^{\pm}_{kl}, k+l\leq i+j-1$.

It is easy to see that for some values of positive numbers ω_1,ω_2 the denominators in expression (3.2) are equal to zero.

In order to solve (2.6) we consider diffeomorphisms

$$\Phi^{\pm}\colon (y_1,y_2)\longmapsto \Big(y_1+\sum_{i+j\geq 2}\Phi^{\pm}_{1,ij}y_1^iy_2^j,\quad y_1+\sum_{i+j\geq 2}\Phi^{\pm}_{1,ij}y_1^iy_2^j\Big) \tag{3.3}$$

which transform the vector fields $\nabla S^{\pm}\bullet\nabla$ to the following normal forms:

$$L_0^{\pm}=\omega_1y_1\frac{\partial}{\partial y_1}\pm\omega_2y_2\frac{\partial}{\partial y_2}\,. \tag{3.4}$$

To formulate the existance theorem we need two definitions.

We say that positive numbers ω_1 and ω_2 are *nonresonant* if they satisfy the following conditions

$$\omega_1\neq k\omega_2,\quad \omega_2\neq k\omega_1,\quad k=2,3,\ldots \tag{3.5}$$

Positive numbers ω_1 and ω_2 are said to be *Diophantine* if there exist positive numbers α and C such that for nonnegative integers i,j, ~~such that~~ $i+j\geq 1$,

$$|i\omega_1-j\omega_2|\geq\frac{C}{(i+j)^{\alpha}} \tag{3.6}$$

Theorem. *Let the potential V be represented by a series of the form (2.1) convergent in a neigbourhood of the origin.*

1. *If numbers ω_1 and ω_2 are nonresonant then there exist a unique positive analytic function S^+ which can be represented by convergent series of the form (3.1) in some neigbourhood of the origin and satisfies the equation (2.6), and an analytic diffeomorphism Φ which transforms vector field $\nabla S^+\bullet\nabla$ to the normal form L_0^+ given by (3.4).*
2. *If the numbers ω_1 and ω_2 are Diophantine then there exist a unique analytic function S^- which can be represented by convergent series of the form (3.1) in some neigbourhood of the origin and satisfies the equation (2.6), and an analytic diffeomorphism Φ^- which transforms vector field $\nabla S^-\bullet\nabla$ to the normal form L_0^- given by (3.4).*

Note 1. The proof of this theorem can be found in [11]. To suppress small denominators wich appear in the series (3.1) and prove the theorem, we use the Newton method with the simultaneous change (3.3) of variables at each step.

Note 2. The analytic at the origin functions ψ_1 and ψ_2 can be found uniquely from the equation (2.7), see [12].

§4. AMPLITUDE COEFFICIENTS AND EIGENVALUES

Here we construct solutions of the equations (2.8), (2.9). The first approximation to an eigenvalue is

$$E_1^{n_1 n_2} = \left(n_1 + \frac{1}{2}\right)\omega_1 + \left(n_2 + \frac{1}{2}\right)\omega_2. \tag{4.1}$$

Let the frequences ω_1, ω_1 be Diophantine.
Then the solution $\vec{\mathcal{A}}_0$ of the system (2.8) can be found in the form

$$\vec{\mathcal{A}}_0 = \Psi J \vec{B}_0, \tag{4.2}$$

where

$$\Psi = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & \frac{1}{\psi_1} & 0 & 0 \\ 0 & 0 & \frac{1}{\psi_2} & 0 \\ 0 & 0 & 0 & \frac{1}{\psi_1 \psi_2} \end{pmatrix}, \tag{4.3}$$

$$J = \frac{1}{2}\begin{pmatrix} 1 & 1 & 1 & 1 \\ 1 & 1 & -1 & -1 \\ 1 & -1 & -1 & 1 \\ 1 & -1 & 1 & -1 \end{pmatrix}, \tag{4.4}$$

$$\vec{B}_0 = \left(B_1^+, B_1^-, B_2^+, B_2^-\right)^T, \tag{4.5}$$

$B_l^\pm = c_l^\pm e^{\mathcal{P}_l^\pm}$, $l = 1, 2$, the functions $\mathcal{P}_l^\pm$ being analytic solutions of the equation

$$L_0^\pm \tilde{\mathcal{P}}_l^\pm = d_l \tilde{\kappa} - \tilde{\theta}^\pm, \; l = 1, 2, \; d_1 = 1, \; d_2 = -1, \tag{4.6}$$

$\tilde{}$ meaning a change of variables, $F(x_1, x_2) = \tilde{F}(y_1, y_2)$,

$$\theta^\pm = \psi_1 \frac{\Delta\psi_1}{2} \pm \psi_2 \frac{\Delta\psi_2}{2}. \tag{4.7}$$

The existance of those solutions in some neighbourhood of the origin is proven in [12]. One can prolong them analytically onto a larger domain by the formula

$S = \int p_1 dx_1 + p_2 dx_2$ where the integral is taken along the trajectory of the corresponding Hamiltonian system (the formulae written in [10]).

One can see that the functions $\mathcal{A}_l^0, l = 2,3,4$, have singularities at the origin (where $\psi_l, l = 1,2$, vanish).

Let us express the functions D_n and their derivatives by Hermitian polinomials H_n and the exponents, we shall find that

$$
\begin{aligned}
u^{[0]}_{n_1,n_2} = e^{-\frac{\psi_1^2+\psi_2^2}{\hbar}} \cdot \{ & H_{n_1}H_{n_2}[\mathcal{A}_1^0 - \psi_1\mathcal{A}_2^0 - \psi_2\mathcal{A}_3^0 + \psi_1\psi_2\mathcal{A}_4^0] \\
& + \sqrt{\hbar}[H'_{n_1}H_{n_2}(\mathcal{A}_2^0 - \psi_2\mathcal{A}_4^0) + H_{n_1}H'_{n_2}(\mathcal{A}_3^0 - \psi_1\mathcal{A}_4^0)] \\
& + \hbar H'_{n_1}H'_{n_2}\mathcal{A}_4^0\} .
\end{aligned} \tag{4.8}
$$

We see that the senior term in respect to $\hbar$ has no singularities. The first multiplier in square brackets is equal to $2B_2^+$ and that is an analytic function accordig to the said above. The functions $\mathcal{A}_2^0 - \psi_2\mathcal{A}_4^0$, $\mathcal{A}_3^0 - \psi_1\mathcal{A}_4^0$ and $\mathcal{A}_4^0$ have singularities (of the type $\frac{1}{\psi_1}$, $\frac{1}{\psi_2}$ and $\frac{1}{\psi_1\psi_2}$ correspondently). These singularities disappear in (4.8) when the quantum numbers n_1 and n_2 are even and they remain when the mentioned numbers are odd.

The presence of the singularities in the case of odd n_1 and n_2 reflects the fact that the equations $\psi_1 = 0$ or $\psi_2 = 0$ do not define the genuine zeros of the eigenfunction u_{n_1,n_2} as it follows formally from (2.3). The genuine zeros are shifted and in general case their lines have no intersections. In fact singularities cancel if one takes into account all subsiquent approximations.

To give an idea how the singularities cancell let us concider for simplicity the case $n_1 = n_2 = 1$.

§5 Quantum numbers 1,1.

In this case $H_1(t) = t, H'_1(t) = 1$, so we have to look for the second approximation of the eigenfunction $u_{1,1}$ and the corresponding eigenvalue in the following form:

$$
u^{[1]}_{1,1} = e^{-\frac{S}{\hbar}}(2\psi_1\psi_2 B + \hbar G). \tag{5.1}
$$

(Here $B = B_2^+ = c_2^+ e^{\mathcal{P}_2^+}$, $\mathcal{P}_2^+$ being a solution of (4.6) ,l=2.)

$$
E^{[2]}_{1,1} = \hbar E_1^{1,1} + \hbar^2 E_2^{1,1}, \tag{5.2}
$$

$$
E_1^{1,1} = \frac{3}{2}\omega_1 + \frac{3}{2}\omega_2. \tag{5.3}
$$

From the Schrödinger equation (1.1) we find the following equation for the function G_2

$$
\begin{aligned}
\nabla S \bullet \nabla G + \left(\frac{\Delta S}{2} - E_1^{1,1}\right) G = & (\psi_2\Delta\psi_1 + \psi_1\Delta\psi_2)B + 2\psi_2\nabla\psi_1 \bullet \nabla B \\
& + 2\psi_1\nabla\psi_2 \bullet \nabla B + \psi_1\psi_2\Delta B + 2E_2^{1,1}\psi_1\psi_2 B.
\end{aligned} \tag{5.4}
$$

Now the function $\varkappa$ defined by (2.11) is the following:

$$\varkappa = \frac{3}{2}(\nabla\psi_1)^2 + \frac{3}{2}(\nabla\psi_2)^2 \tag{5.5}$$

(it depends on n_1, n_2). So

$$\frac{\Delta S}{2} - E_1^{1,1} = \theta + \varkappa - (\nabla\psi_1)^2 - (\nabla\psi_2)^2, \tag{5.6}$$

(θ is defined by (4.7) with sign +). One can see that

$$\left(\theta + \varkappa - (\nabla\psi_1)^2 - (\nabla\psi_2)^2\right)\big|_{(0,0)} = -\omega_1 - \omega_2. \tag{5.7}$$

Finding the function G.

We consider at first the corresponding homogeneous equation with the change pf variables (3.3) (with sign +):

$$L_0\tilde{G}^0 + \left(\tilde{\theta} + \tilde{\varkappa} - (\nabla\tilde{\psi}_1)^2 - (\nabla\tilde{\psi}_2)^2\right)\tilde{G}^0 = 0, \tag{5.8}$$

L_0 defined by (3.4). We look for the solution of (5.8) in the following form:

$$\tilde{G}^0 = y_1 y_2 e^{\tilde{\mathcal{P}}} \tag{5.9}$$

and find the equation for $\tilde{\mathcal{P}}$

$$L_0\tilde{\mathcal{P}} = (\nabla\tilde{\psi}_1^2) + (\nabla\tilde{\psi}_2^2) - \tilde{\theta} - \tilde{\varkappa} - (\omega_1 + \omega_2) \tag{5.10}$$

with the right-hand side vanishing at the origin. Due to Lemma 3.1 of [2] there exists a unique analytic solution of (5.10) vanishing at the origin. Let $\tilde{\mathcal{P}}$ be that solution.

Now we look for the solution of (5.4) (in variables y_1, y_2) in the following form

$$\tilde{G} = \tilde{U}e^{\tilde{\mathcal{P}}} = \frac{\tilde{U}}{y_1 y_2} y_1 y_2 e^{\tilde{\mathcal{P}}}. \tag{5.11}$$

Putting (5.11) in (5.4) we obtain the following equation for the function $\tilde{U}$

$$L_0\tilde{U} - \omega_1\tilde{U} - \omega_2\tilde{U} = \tilde{F}e^{-\tilde{P}}, \tag{5.12}$$

by F is denoted the right-hand side of the equation (5.4).

Lemma. *If the right-hand side of (5.12) is analytic and its second mixed partial derivative with respect to y_1, y_2 wanishes at the origin then there exists a unique analytic solution of (5.12) also with the wanishing at the origin second mixed partial derivative with respect to y_1, y_2.*

This lemma can be proven mainly in the same way as Lemma 3.1 in [2]

The second term of the eigenvalue.

The condition of solvability of the equation (5.12), given by the Lemma, reads:

$$\left(\tilde{F}e^{-\tilde{\mathcal{P}}}\right)_{11} = 0, \tag{5.13}$$

where $(u)_{ij}$ means the i,j–th Taylor coefficient of the function $u(\vec{y})$.

We can satisfy this condition with the corresponding choice of E_2^{11}, that is

$$\begin{aligned} E_2^{11} &= -\frac{(\Delta\tilde{B})_{00}}{2} \\ &- \frac{1}{\sqrt{\omega_1\omega_2}}\left(e^{-\tilde{\mathcal{P}}}\left[\tilde{\psi}_2(\frac{\Delta\tilde{\psi}_1}{2}) + \tilde{\psi}_1(\frac{\Delta\tilde{\psi}_2}{2})\tilde{B} + \tilde{\psi}_2\nabla\tilde{\psi}_1 \bullet \nabla\tilde{B} + \tilde{\psi}_1\nabla\tilde{\psi}_2 \bullet \nabla\tilde{B}\right]\right)_{11}, \end{aligned} \tag{5.14}$$

where ψ_1, ψ_2, $\mathcal{P}$ and B are mentioned above functions (the corresponding Taylor coefficients in the right-hand side are writen out in [13] in terms of Taylor coefficients of V).

Zeros of the eigenfunction.

The equation of the line of the zeros of the eigenfunction u_{11} is the following

$$2\psi_1\psi_2 e^{\mathcal{P}_2^+} + \hbar U e^{\mathcal{P}} = 0. \tag{5.15}$$

It is clear that $(U)_{00} = 0$ (because $F(0,0) = 0$, see (5.4)). The first Taylor coefficients $(U)_{10}$ and $(U)_{01}$ of U can be found from (5.12). They are

$$(U)_{10} = \frac{1}{\sqrt{\omega_1}}[(\psi_2)_{20} + (\psi_2)_{02}] + 2\sqrt{\frac{\omega_2}{\omega_1}}(\mathcal{P}_2^+)_{01}, \tag{5.16}$$

$$(U)_{01} = \frac{1}{\sqrt{\omega_2}}[(\psi_1)_{20} + (\psi_1)_{02}] + 2\sqrt{\frac{\omega_1}{\omega_2}}(\mathcal{P}_2^+)_{10}, \tag{5.17}$$

the right-hand sides (writen out in [13]) depend on ω_1, ω_2 and v_{ij}, $i + j = 3$, and do not vanish at the origin in general case. So in the zero approximation the lines of zeros of $u_{1,1}$, namely

$$\begin{aligned} \psi_1 &= 0, \\ \psi_2 &= 0, \end{aligned} \tag{5.18}$$

intersect at the origin. In the next approximation they split into the two branches of a hyperbola in a neighbourhood of the origin:

$$2\sqrt{\omega_1\omega_2}x_1x_2 + \hbar\left[(U)_{10}x_1 + (U)_{01}x_2\right] = 0. \tag{5.19}$$

One of these branches goes through the origin. In general case these lines do not intersect. They have only a "quasi-intersection".

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