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Semi-classical eigenstates at the bottom of a multidimensional well

by

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ABSTRACT. – The Schrödinger operator in $\mathbb{R}^d$ with an analytic potential, having a nondegenerated minimum (well) at the origin, is considered. Under a Diophantine condition on the frequencies, the full asymptotic series (the Plank constant $\hbar$ tending to zero) for a set of eigenfunctions and eigenvalues in some zone above the minimum is constructed; the Gaussian-like asymptotics being valid in a neighbourhood of the origin which is independent of $\hbar$.

RÉSUMÉ. – On considère l'opérateur de Schrödinger dans $\mathbb{R}^d$, avec un potentiel analytique possédant un minimum (puits) non-dégénéré à l'origine. Moyennant une condition diophantienne sur les fréquences, on construit une série asymptotique complète en $\hbar$ ($\hbar$ tendant vers zéro) pour les fonctions et les nombres propres concentrés au fond du puits (de vecteurs quantiques $n \in \mathbb{N}^d$ donnés); les estimations asymptotiques de type gaussien étant valables dans un voisinage de l'origine qui est indépendant de $\hbar$.

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1. INTRODUCTION

We consider the Schrödinger equation

$$-\frac{\hbar^2}{2}\,\Delta u + V\,u = E\,u, \tag{1.1}$$

where $\Delta = \sum_{i=1}^{d} \frac{\partial^2}{\partial x_i^2}$ is the Laplace operator, V is a real valued function defined on $\mathbb{R}^d$ having a nondegenerated minimum at the origin.

We are interested in the semiclassical ($\hbar \to 0$) asymptotics of the discrete spectrum of the Schrödinger operator defined by the left hand side of the equation (1.1) 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 and $V(x) > C$ beyond the region of the wells where C exceeds the value of V at minimum, lower part of the spectrum of the corresponding Schrödinger operator is organized in the following way. There is a set of finite groups of eigenvalues (each of them connected with some quantum vector $n \in \mathbb{N}^d$), 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 $\hbar$.

It is possible to find explicit formulae for the widths of these splittings semiclassical asymptotics for each well. The problem was considered in different ways by different authors and almost completely solved in one dimensional case ([1]-[11]). The case $d > 1$ seems much more complicated. There are many results obtained in this area up to now (*see* [11]-[20] and the list is far not full). Still the picture is not so complete as when $d = 1$. The semiclassical asymptotics of the descrete spectrum and strict estimates of the splittings are described in [11]-[13] and other works of these authors (using the theory of pseudo differential operators). The semiclassical expansion for the eigenfunctions and the rigourous asymptotics for the splitting widths in the lowest levels ($n = 0$) were obtained in [18]-[20] (with the use of a tunnel canonical operator). Still there are no effective (as when $d = 1$) splitting asymptotic formulae in terms of potential for a set of arbitrary levels ($|n| = 1,\ 2,\ 3,\ \ldots$). The mentioned methods do not allow to obtain them.

In order to write down the strict asymptotic formulae for the splittings in the d-dimensional case developing the methods of [9] it is necessary to find a sufficiently accurate semiclassical approximation to eigenstates for a single well in some neighbourhood of a minimum, independent of $\hbar$. The main aim of the present paper is to construct such an approximation. We obtain the formal series on powers of $\hbar$. Coefficients in all terms are found in some domain independent of $\hbar$. Terms for eigenfunctions are analytic for analytic potential. If we truncate the series at the N-th term the remaining sums satisfy the equation (1.1) with the error of order $\hbar^{N+1} e^{-\frac{S}{\hbar}}$, where S is a nonnegative function defined later. They give us so called *quasi-modes* [21]. The possibility to take N as large as we like and exponential decreasing of all terms beyond some neighbourhood of a minimum allows one to hope that, with the help of *quasi-modes*, it is possible to find real eigenfunctions and eigenvalues approximately, with exponentially small errors, smaller than the widths of splittings, so as to be able to find these widths with sufficient accuracy. (The program was realized in [9] for $d = 1$.) The constructed series allow to investigate the set of zeros of the eigenfunctions. The latter is interesting by itself and may be essentially used while finding the splitting asymptotics for $|n| \geq 1$.

2. ASYMPTOTIC EXPANSIONS FOR THE EIGENSTATES

We look for eigenfunctions u_n and eigenvalues E_n of (1.1) in the form of the following series

$$E_n = \sum_{j=1}^{\infty} E_{nj} \hbar^j, \tag{2.1}$$

$$u_n = \exp\left\{-\frac{S}{\hbar}\right\} \sum_{j=0}^{\infty} u_{nj} \hbar^j, \tag{2.2}$$

where $E_{n_i} \in \mathbb{R}$, $n = (n_1, n_2, \ldots, n_d) \in \mathbb{N}^d$ is a quantum vector, $S = S(x)$, $x = (x_1, x_2, \ldots, x_d) \in \mathbb{R}^d$, $u_{nj} = u_{nj}(x)$, $j = 0\ 1,\ 2, \ldots,$ are functions independent of $\hbar$.

We look u_{n0} in the following form

$$u_{n0} = \psi^n e^{\mathcal{P}_n(x)}, \tag{2.3}$$

where $\mathcal{P}_n(x)$ is an unknown function (to be found later),

$$\psi = \psi(x) = (\psi_1(x), \psi_2(x), \ldots, \psi_d(x)), \qquad \psi^n = \prod_{i=1}^{d} \psi_i^{n_i},$$

the functions $\psi_i(x)$, $i = 1, 2, \ldots, d$, and $S(x)$ satisfy the following equations

$$S(x) = S^0(x) = \frac{1}{2}\sum_{i=1}^{d}\psi_i^2, \tag{2.4}$$

$$S^j = \frac{1}{2}\sum_{i=1}^{d}(1 - 2\,\delta_{ij})\,\psi_i^2, \qquad j = 1, \ldots, d,$$

$$\delta_{ij} = \begin{cases} 1, & \text{if } i = j, \\ 0, & \text{if } i \neq j, \end{cases} \tag{2.5}$$

$$(\nabla S^j)^2 = 2\,V, \qquad j = 0, 1, \ldots, d, \tag{2.6}$$

$$\langle \nabla \psi_i, \nabla \psi_j \rangle = \delta_{ij}\,(\nabla \psi_j)^2. \tag{2.7}$$

Symbols ∇ and $\langle \cdot, \cdot \rangle$ denote a *gradient* and a *scalar product* in $\mathbb{R}^d$ respectively.

We put the series (2.1) and (2.2) into the Schrödinger equation (1.1) and equate coefficients of each power of $\hbar$ to zero. The equation for power 0 is satisfied automatically because of (2.6). The requirement for the coefficient of first degree in $\hbar$ to be equal to zero gives us the following equation for the function $\mathcal{P}_n$ and the number E_{n1}:

$$\langle \nabla S^0, \nabla \mathcal{P}_n \rangle = E_{n1} - \frac{\Delta S^0}{2} - \sum_{i=1}^{d} n_i\,(\nabla \psi_i)^2. \tag{2.8}$$

The analogous requirement for the coefficient of $\hbar^2$ gives the equation for u_{n1} and E_{n2}:

$$\langle \nabla S^0, \nabla u_{n1} \rangle + \left(\frac{\Delta S^0}{2} - E_{n1}\right) u_{n1} = \left\{F_1 + \psi^n \left[\frac{\Delta \mathcal{P}_n + (\nabla \mathcal{P}_n)^2}{2} + E_{n2}\right]\right\} e^{\mathcal{P}_n}, \tag{2.9}$$

where

$$F_1 = \sum_{i=1}^{d} \frac{n_i (n_i - 1)}{2} \psi_i^{n_i - 2} (\nabla \psi_i)^2 \prod_{j \neq i} \psi_j^{n_j} + \sum_{i=1}^{d} \frac{n_i}{2} \psi_i^{n_i - 1} \Delta \psi_i \prod_{j \neq i} \psi_j^{n_j} + \sum_{i=1}^{d} n_i \psi_i^{n_i - 1} \langle \Delta \psi_i, \nabla \mathcal{P}_n \rangle \prod_{j \neq i} \psi_j^{n_j}. \tag{2.10}$$

So on, for each $j \geq 2$ we obtain the equation

$$\langle \nabla S^0, \nabla u_{nj} \rangle + \left(\frac{\Delta S^0}{2} - E_{n1} \right) u_{nj} = \frac{\Delta u_{n,\,j-1}}{2} + \sum_{l=1}^{j-1} E_{n,\,l+1}\, u_{n,\,j-l} + \psi^n\, e^{\mathcal{P}_n (x)}\, E_{n,\,j+1}. \tag{2.11}$$

In sections 3 and 4 we will formulate and prove an existence theorem for (2.6); in section 5 we will find all the functions $\psi_i (x)$, $i = 1, 2, \ldots, d$, and $u_{nj} (x)$, $j = 0, 1, 2, \ldots$, all the numbers E_{nj}, $j = 1, 2, \ldots$, for some set of n in some neighbourhood of the origin, independent of $\hbar$. In section 6 we will formulate a concluding theorem and make concluding remarks.

3. THE PHASE THEOREM FOR THE ANALYTIC POTENTIAL

Let V be analytic with the following Taylor series

$$V(x) = \frac{1}{2} \sum_{i=1}^{d} \omega_i^2 x_i^2 + \sum_{|k| \geq 3} v_k x^k, \qquad k = (k_1, k_2, \ldots, k_d) \in \mathbb{N}^d, \qquad |k| = \sum_{i=1}^{d} k_i, \tag{3.1}$$

convergent in a polydisk $|x_i| \leq r$, $i = 1, 2, \ldots, d$ with the numbers $\omega_i > 0$, $i = 1, 2, \ldots, d$.

We search solutions of the equation (2.6) in the form of the following power series

$$S^j(x) = \frac{1}{2} \sum_{i=1}^{d} \omega_i (1 - 2\delta_{ij})\, x_i^2 + \sum_{|k| \geq 3} (S^j)_k\, x^k, \tag{3.2}$$
$$j = 0, 1, \ldots, d.$$

Substituting (3.2) in (2.6) and comparing coefficients of x^k we find the following recurrent formulae for $(S^j)_k$:

$$(S^j)_k = \frac{\tilde{v}_k}{\langle k, I_j\, \omega\rangle}, \tag{3.3}$$

where $\omega = (\omega_1, \omega_2, \ldots, \omega_d)$; I_0 is a unitary matrix of order d; I_j, $j = 1, \ldots, d$, is a diagonal matrix of the order d with -1 standing at the j-th place of the diagonal and 1 at the others,

$$\tilde{v}_k = v_k \qquad \text{for} \quad |k| = 3$$

and

$$\tilde{v}_k = v_k + \text{terms, depending on } (S^j)_\kappa, \qquad |\kappa| < |k| \quad \text{for } |k| \geq 4.$$

It is easy to see that for the positive numbers ω_i, $i = 1, 2, \ldots, d$, the denominators in expressions (3.3) for $j = 1, 2, \ldots, d$, can be equal to zero. So even to construct these series formally we have to propose some additional conditions on the potential V.

Simultaneously we will construct a change of variables

$$\Phi^j : \quad y_j = (y_{j1}, \ldots, y_{jn}) \mapsto (x_1 = \Phi_1^j(y_j), \ldots, x_d = \Phi_d^j(y_j)), \tag{3.4}$$

which transforms the vector field $\langle \nabla S^j, \nabla \cdot \rangle$ into the normal form

$$L_0^j = \sum_{i=1}^{d} \omega_i (1 - 2\delta_{ij})\, y_{ji} \frac{\partial}{\partial y_{ji}}. \tag{3.5}$$

We search the functions $\Phi_i^j(y)$, $i = 1, 2, \ldots, d$ in the following form

$$\Phi_i^j(y_j) = y_{ji} + \sum_{|k| \geq 2} (\Phi_i^j)_k\, y_j^k. \tag{3.6}$$

In order to find the coefficients $(\Phi_i^j)_k$ we replace x_i, $i = 1, 2, \ldots, d$, in $\langle \nabla S^j, \nabla \cdot \rangle$ by $\Phi_i^j(y_i)$ of the form (3.6) and equate the obtained series (in variables y) to L_0^j. Hence we find the following expressions for the coefficients

$$(3.7) \qquad (\Phi_i^j)_k = \frac{\tilde{S}_{i,j,k}}{\langle k - \mathrm{ort}_i, I_j\, \omega \rangle}, \qquad j = 0, 1, \ldots, d, \quad |k| \geq 2,$$

where

$$\tilde{S}_{i,j,k} = (k_i + 1)\,(S^j)_{k - \mathrm{ort}_i} + \text{terms, depending on } (\Phi_l^j)_\kappa,$$
$$l = 1, 2, \ldots, d, \quad |\kappa| < |k|,$$

ort_i is an element of a standard basis $\{\mathrm{ort}_i\}_1^d$ having all components equal to 0 except of the i-th one which is equal to 1.

We see here that some denominators are equal to zero for some values of ω. We have to exclude these values.

Let us make the following definitions.

We say, that the positive numbers $\omega_1, \omega_2, \ldots, \omega_d$ are *nonresonant* if they are linearly independent over integers.

Positive numbers $\omega_1, \omega_2, \ldots, \omega_d$ are said to be *Diophantine* if there exist positive numbers α and C such that for any $k \in \mathbb{Z}^d$, $k \neq 0$,

$$(3.8) \qquad |\langle k, \omega \rangle| \geq \frac{C}{|k|^\alpha}.$$

Denote the set of vectors $\omega = (\omega_1, \omega_2, \ldots, \omega_d)$ with positive components by Ω, the set of ω with nonresonant components by Ω_{nr}, the set of ω with Diophantine components by Ω_D.

THEOREM A. – *Let the potential V be analytic, represented by a series of the form* (3.1) *convergent in a neighbourhood of the origin.*

(1) *If $\omega \in \Omega_{\mathrm{nr}}$ then there exists a pair: a unique positive analytic function S^0 which can be represented by convergent series of the form* (3.2) *for $j = 0$ in some neighbourhood of the origin and satisfies the equation* (2.6); *and a unique analytic diffeomorphism Φ^0 which transforms the vector field $\langle \nabla S^0, \nabla \cdot \rangle$ to the normal form L_0^0 given by* (3.5).

(2) *If $\omega \in \Omega_D$ then for each $j \in (1, 2, \ldots, d\}$ there exists a pair: a unique analytic function S^j which can be represented by convergent series of the form* (3.2) *in some neighbourhood of the origin and satisfies the equation*

(2.6); *and a unique analytic diffeomorphism* Φ^j *which transforms the vector field* $\langle \nabla S^j, \nabla \cdot \rangle$ *to the normal form* L_0^j *given by* (3.5).

This theorem will be proven in the next section.

Remark 3.1. – Normal forms of the vector fields (*i.e.* of hamiltonian systems of differential equations) are described in literature on classical mechanics e.g. [22]-[25]. A typical situation there is that given a vector field one has to find the simpliest form for it in suitable variables. Here we have no given vector fields. We are looking for vector fields which are solutions of the nonlinear Eiconal equation (2.6). The normal forms (3.5) are used as an auxiliary tool.

Remark 3.2. – In case (1) the nonresonance condition is necessary to construct Φ^0 (not S^0). There are no small denominators in (3.3) for $j = 0$. The existence of analytic S^0 was established in [26] in more general situation.

Remark 3.3. – One can give the following geometrical interpretation to the results of the theorem A. The functions S^j are the generating functions for Lagrangian manifolds which are invariant with respect to the classical dynamical system with the potential $-V(x)$. The potential $-V(x)$ has a "hunch" at the origin (instead of a "well" of $V(x)$). So our quantum mechanical problem "at the bottom of a well" is equivalent to a classical problem "near the top of a hill". The origin is a point of singularity in this problem, a point of the infinite time in classical dynamics, a point of vanishing energy of the Lagrangian manifolds. The theorem gives the existence of the generating functions S^j for the invariant Lagrangian manifolds in a small neighbourhood of that point.

The geometrical aspects of the problem were considered in [27].

4. THE PROOF OF THE THEOREM. NEWTON'S METHOD

To suppress small denominators which appear in the series (3.2) we use the Newton method (*see* e.g. [27]). Since the proof goes in a similar way for all $j = 0, 1, 2, \ldots, d$ we will omit the index j at a function S^j and a map Φ^j (and hence at a point y_j and a variable y_{ji}).

We have to find a function

$$S: \quad \mathcal{G} \mapsto \mathbb{C}$$

and a diffeomorphism

$$\Phi: \quad B(r) \mapsto \mathcal{G},$$

where $\mathcal{G}$ is a neighbourhood of the origin in $\mathbb{C}^d$,

$$B(r) = \{y \in \mathbb{C}^d : |y_i| < r,\ i = 1, 2, \ldots, d\} \tag{4.1}$$

such that:

S is holomorphic, its Taylor series is of the form (3.2) and it satisfies the equation (2.6); the map Φ is holomorphic and conjugates the vector field L_0 defined on $B(r)$ with $\langle \nabla S, \nabla \cdot \rangle$ defined on $\mathcal{G}$.

As a starting approximation we take the function

$$S^{(0)} = \frac{1}{2} \sum_{i=1}^{d} \omega_i (1 - 2\delta_{ij}) x_i^2 + \sum_{|k|=3}^{N} (S^j)_k x^k, \tag{4.2$^{(0)}$}$$

where the coefficients $(S^j)_k$ are defined by the recurrent relations (3.3), and the map

$$\Phi^{(0)} : B(r^{(0)}) \mapsto \mathcal{G}^{(0)} = \Phi^{(0)}(B(r^{(0)}), \tag{4.3$^{(0)}$}$$

given by the formula

$$\Phi(y) = \left(y_1 + \sum_{|k|=2}^{N} (\Phi_1)_k y^k,\ y_2 + \sum_{|k|=2}^{N} (\Phi_2)_k y^k,\ \ldots,\ y_d + \sum_{|k|=2}^{N} (\Phi_d)_k y^k \right), \tag{4.4$^{(0)}$}$$

where the coefficients $(\Phi_i)_k$ are defined in (3.7). The function $S^{(0)}$ satisfies the equation (2.6) with an error $\Upsilon^{(0)}$:

$$\frac{1}{2} (\nabla S^{(0)})^2 = V + \Upsilon^{(0)}, \tag{4.5$^{(0)}$}$$

and the map $\Phi^{(0)}$ conjugates the vector fields L_0 and $\langle \nabla S, \nabla \cdot \rangle$ also with an error (defined by $\mu_i^{(0)}$ in the i-th component):

$$(\Phi^{(0)})_*^{-1} \langle \nabla S^{(0)}, \nabla \cdot \rangle = \sum_{i=1}^{d} (\omega_i (1 - 2\delta_{ij}) y_i + \mu_i^{(0)}) \frac{\partial}{\partial y_i}. \tag{4.6$^{(0)}$}$$

One can notice that the Taylor expansion for $\Upsilon^{(0)}$ contains a power term with x^k if and only if $|k| \geq N + 1$, and those for $\mu_i^{(0)}$, $i = 1, 2, \ldots, d$, contain the terms y^k only with $|k| \geq N$.

We fix a sufficiently large $N > 4(\alpha + d + 1)$ and choose $r^{(0)}$ so that the error terms in ($4.5^{(0)}$) and ($4.6^{(0)}$) satisfy the estimate

$$(4.7^{(0)}) \qquad \max_{1 \le i \le d} \{\|\Upsilon^{(0)}\|, \|\mu_i^{(0)}\|\} \le \varepsilon^{(0)},$$

where

$$\|f^{(n)}\| = \sup_{y \in B(r^{(n)})} |f^{(n)}(y)|,$$

and $\varepsilon^{(0)}$ is a small constant which we will fix later.

Let us describe a typical step of the Newton method. Suppose that on the n-th step we have a function

$$S^{(n)} : \mathcal{G}^{(n)} \mapsto \mathbb{C}$$

and a diffeomorphism

$$\Phi^{(n)} : B(r^{(n)}) \mapsto \mathcal{G}^{(n)} = \Phi^{(n)}(B(r^{(n)}) \ni (0, 0, \ldots, 0),$$

where $B(r^{(n)})$ is the polydisk of the form (4.1) with the radius

$$(4.8) \qquad r^{(n)} = r^{(0)} - \frac{r^{(0)}}{10} \sum_{i=1}^{n-1} \frac{1}{(i+1)^2},$$

such that they satisfy the equations with the error terms $\Upsilon^{(n)}$ and $\mu_i^{(n)}$:

$$(4.5^{(n)}) \qquad \frac{1}{2}(\nabla S^{(n)})^2 = V + \Upsilon^{(n)},$$

$$(4.6^{(n)}) \qquad (\Phi^{(n)})_*^{-1} \langle \nabla S^{(n)}, \nabla \cdot \rangle = \sum_{i=1}^{d} (\omega_i (1 - 2\delta_{ij}) y_i + \mu_i^{(n)}) \frac{\partial}{\partial y_i},$$

the latters obeying the estimate

$$(4.7^{(n)}) \qquad \max_{1 \le i \le d} \{\|\Upsilon^{(n)}\|, \|\mu_i^{(n)}\|\} \le \varepsilon^{(n)}.$$

Suppose by induction that the Taylor series for $\Upsilon^{(n)}$ contains terms with x^k only if $|k| \ge N + 1$, and those for $\mu_l^{(n)}$, $l = 1, 2, \ldots, d$, contain the terms y^k only with $|k| \ge N$.

To find the function of $(n + 1)$-th step we set

$$(4.9) \qquad \Phi^{(n+1)} = \Phi^{(n)} \circ \Psi^{(n)},$$

$$(0,\, 0,\, \ldots,\, 0) \in \mathcal{G}^{(n+1)} = \Phi^{(n)}\left(B\left(r^{(n+1)}\right)\right) \subset \mathcal{G}^{(n)} \tag{4.10}$$

where

$$\Psi^{(n)} : B\left(r^{(n+1)}\right) \mapsto B\left(r^{(n)}\right) \tag{4.11}$$

is a holomorphic map close to identity which is a diffeomorphism onto its image;

$$S^{(n+1)} = S^{(n)}|_{\mathcal{G}^{(n+1)}} + \sigma^{(n)}. \tag{4.12}$$

We will try to find $\sigma^{(n)}$ and $\Psi^{(n)}$ as solutions of linear problems so that new error terms become as small as possible. Let us write out formulae for the new error terms. The equation $(4.5^{(n)})$ reads:

$$\begin{aligned} \Upsilon^{(n+1)} &= \frac{1}{2}(\nabla S^{(n+1)})^2 - V \\ &= \frac{1}{2}(\nabla S^{(n)})^2 - V + \langle \nabla S^{(n)},\, \nabla \sigma^{(n)} \rangle + \frac{1}{2}(\nabla \sigma^{(n)})^2 \\ &= \Upsilon^{(n)} + \langle \nabla S^{(n)},\, \nabla \sigma^{(n)} \rangle + \frac{1}{2}(\nabla \sigma^{(n)})^2. \end{aligned} \tag{4.13}$$

It is convenient to pass to the coordinates

$$y = (\Phi^{(n)})^{-1}(x).$$

We have

$$\begin{aligned} \Upsilon^{(n+1)} \circ \Phi^{(n)} &= \Upsilon^{(n)} \circ \Phi^{(n)} + L_0^j\, \tilde{\sigma}^{(n)} \\ &\quad + \sum_{i=1}^{d} \mu_i^{(n)} \frac{\partial \tilde{\sigma}^{(n)}}{\partial y_i} + \frac{1}{2}(\nabla \sigma^{(n)})^2 \circ \Phi^{(n)} \end{aligned} \tag{4.14}$$

where $\tilde{\sigma}^{(n)} = \sigma^{(n)} \circ \Phi^{(n)}$ and L_0^j is given by (3.5).

If the function $\tilde{\sigma}^{(n)}$ satisfies the linear equation

$$L_0^j\, \tilde{\sigma}^{(n)} = -\Upsilon^{(n)} \circ \Phi^{(n)} \tag{4.15}$$

then the $(n+1)$-th error term becomes "quadratic":

$$\Upsilon^{(n+1)} \circ \Phi^{(n)} = \sum_{i=1}^{d} \mu_i^{(n)} \frac{\partial \tilde{\sigma}^{(n)}}{\partial y_i} + \frac{1}{2}(\nabla \sigma^{(n)})^2 \circ \Phi^{(n)}. \tag{4.16}$$

To find the correction to the transformation $\Phi^{(n)}$ we write (4.6$^{(n+1)}$) which determines $\mu_i^{(n+1)}$, $i = 1, 2, \ldots, d$, in the form

$$\sum_{i=1}^{d} (\omega_i (1 - 2\,\delta_{ij})\,\eta_i + \mu_i^{(n+1)}) \frac{\partial}{\partial \eta_i} = (\Phi^{(n+1)})_*^{-1} [\langle \nabla S^{(n)}, \nabla \cdot \rangle + \nabla \sigma^{(n)}, \nabla \cdot \rangle]. \tag{4.17}$$

We used the notations η_i, $i = 1, 2, \ldots, d$, for the normal coordinates on the $(n+1)$-th step. It follows from (4.9) that

$$(\Phi^{(n+1)})_*^{-1} = (\Psi^{(n)})_*^{-1} \circ (\Phi^{(n)})_*^{-1}. \tag{4.18}$$

Substituting (4.18) into the right hand side of (4.17) and taking into account (4.6$^{(n)}$) one obtains

$$\begin{aligned} \sum_{i=1}^{d} (\omega_i (1 - 2\,\delta_{ij})\,\eta_i + \mu_i^{(n+1)}) \frac{\partial}{\partial \eta_i} &= (\Psi^{(n)})_*^{-1} \left[\sum_{i=1}^{d} (\omega_i (1 - 2\,\delta_{ij})\; y_i + \mu_i^{(n)}) \frac{\partial}{\partial y_i} \right. \\ &\qquad \left. + \langle \nabla \sigma^{(n)}, \nabla \cdot \rangle \circ (\Phi^{(n)}) \right]. \end{aligned} \tag{4.19}$$

To write down explicity the connection between $\mu_i^{(n+1)}$ and $\mu_i^{(n)}$, $i = 1, 2, \ldots, d$, let us denote

$$\eta = (\eta_1, \ldots, \eta_2) = (\Psi^{(n)})^{-1} (y) = (y_1 + \rho_1^{(n)} (y), \ldots, y_d + \rho_d^{(n)} (y)).$$

Then the mentioned connection reads, as it follows from (4.19):

$$\begin{aligned} \mu_i^{(n+1)} \circ (\Psi^{(n)})^{-1} &= -(1 - \delta_{ij})\,\omega_i\,\rho_i^{(n)} + \mu_i^{(n)}) + \hat{\sigma}_i^{(n)} \\ &+ \sum_{l=1}^{d} \left[\omega_l (1 - 2\,\delta_{lj})\; y_l \frac{\partial \rho_i^{(n)}}{\partial y_l} + \mu_l^{(n)} \frac{\partial \rho_i^{(n)}}{\partial y_l} \right], \\ & i = 1, 2, \ldots, d, \end{aligned} \tag{4.20}$$

where

$$\hat{\sigma}_i^{(n)} = \frac{\partial \sigma^{(n)}}{\partial x_i} \circ (\Phi^{(n)}), \qquad i = 1, 2, \ldots, d, \tag{4.21}$$

Again we choose $\rho_i^{(n)}$ so that the "linear" terms in (4.20) cancel. It gives the equations:

$$L_i^j \rho_i^{(n)} = -\mu_i^{(n)} - \hat{\sigma}_i^{(n)}, \qquad i = 1, 2, \ldots, d, \tag{4.22}$$

where

$$L_i^j = -(1 - \delta_{ij})\,\omega_i + L_0^j, \qquad i = 1, 2, \ldots, d, \tag{4.23}$$

L_0^j defined in (3.5).

If $\rho_i^{(n)}$, $i = 1, 2, \ldots, d$, satisfy (4.22) then the new error terms acquire the form:

$$\mu_i^{(n+1)} \circ (\Psi^{(n)})^{-1} = \sum_{l=1}^{d} \mu_l^{(n)} \frac{\partial \rho_i^{(n)}}{\partial y_l}, \qquad i = 1, 2, \ldots, d, \tag{4.24}$$

The equations (4.15) and (4.22) are of the similar type having a bit different operators in the left hand sides. To the similar type belong the equations (2.9), (2.11) for the amplitude coefficients. So now it is convenient to widen the set of operators L_i^j to

$$L_n^j = -\langle I_j\,\omega,\, n\rangle + L_0^j, \tag{4.25}$$

where I_j is the same matrix as in (3.3), $n \in \mathbb{N}^d$, and prove some lemma of solvability for all these equations.

Denote by $\mathcal{B}_r$ a Banach space of analytic functions in $B(r)$ (*see* (4.1)) with the norm

$$\|f\| = \sup_{y \in B(r)} |f(y)|, \tag{4.26}$$

by $\mathcal{B}_{r,M,n,0}$ the subspace of $\mathcal{B}_r$ which is the set of functions having the Taylor series which contains only the terms with power $|k| \geq M \geq 0$ and with coefficient at power n equal to zero, by $\omega_0 = \min_{i \in \{1, \ldots, d\}} \omega_i$.

LEMMA 1. – *Given $r' < r$, there exists a bounded operator* $\{L_n^j\}^{-1}$

$$\{L_n^j\}^{-1} : \mathcal{B}_{r,\, M,\, n,\, 0} \to \mathcal{B}_{r',\, M,\, n,\, 0} \tag{4.27}$$

which solves the equation

$$L_n^j\, u = f|_{B\,(r')}, \qquad u \in \mathcal{B}_{r',\, M,\, n,\, 0}, \quad f \in \mathcal{B}_{r,\, M,\, n,\, 0}. \tag{4.28}$$

in the following cases

(1) *for any* $\omega \in \Omega$, $j = 0$, $n = (0, \ldots, 0)$,

(2) *for* $\omega \in \Omega_{\mathrm{nr}}$, $j = 0$, *n arbitrary,*

(3) *for* $\omega \in \Omega_D$, $j = 1, \ldots, d$, *n arbitrary,*

and there exists a positive constant $c_1 = c_1\,(M,\ d,\ \omega,\ r)$ *such that in both cases* (1), (2):

$$\|\{L_n^0\}^{-1}\| \le \frac{c_1}{(r - r')^{d-1}}, \tag{4.29}$$

in case (3) *there exists a positive constant* $c_2 = c_2\,(\alpha,\ M,\ d,\ \omega,\ r)$ *such that*

$$\|\{L_n^j\}^{-1}\| \le \frac{c_1}{(r - r')^{\alpha+d}}. \tag{4.30}$$

Proof. – Consider the equation (4.28) with f having the following convergent series in $B\,(r)$

$$f\,(y) = \sum_{|k| \ge M} f_k\, y^k \tag{4.31}$$

and let us search the solution of this equation as a power series

$$f\,(y) = \sum_{|k| \ge 0} f_k\, y^k. \tag{4.32}$$

From the equation (4.28) we find the following formulae for the coefficients u_k

$$u_k = \frac{f_k}{\langle I_j\, \omega,\ k - n\rangle}\bigg|_{k \ne n}, \ u_n = f_n = 0, \qquad u_k|_{|k|<M} = 0. \tag{4.33}$$

Hence we find the following estimate for $k \neq n$

$$u_k \leq \frac{|f_k|}{|k-n|\,\omega_0} \leq \frac{c|f_k|}{|k|\,\omega_0} \leq \frac{c\,||f||}{|k|\,\omega_0\, r^k}, \tag{4.34}$$

in the cases (1), (2) and

$$|u_k| \leq \frac{|k|^\alpha\,|f_k|}{C} \leq \frac{|k|^\alpha ||f||}{C\, r^k} \tag{4.35}$$

in the cases (3). The last inequalities in (4.34) and (4.35) come from the Cauchy formula. Therefore we get the estimate

$$\begin{aligned} ||u|| &\leq |\sum_{|k|\geq M} u_k\, y^k| \leq c \sum_{l \geq M} (l+d-2)\dots(l+1)\left(\frac{r'}{r}\right)^l ||f|| \\ &\leq \frac{c_1}{(r-r')^{d-1}}\,||f|| \end{aligned} \tag{4.36}$$

in cases (1), (2), and

$$||u|| \leq c \sum_{l\geq M} l^\alpha\,(l+d-1)\dots(l+1)\left(\frac{r'}{r}\right)^l ||f|| \leq \frac{c_2}{(r-r')^{\alpha+d}}\,||f|| \tag{4.37}$$

in case (3) which ends the proof of lemma 1. □

Remark. – It is clear that the estimates for the norms of the first derivatives of u differ from (4.36), (4.37) by a multiplier $(r-r')^{-1}$.

We apply Lemma to the equation (4.15) taking $M = N+1$ and to the equation (4.22) with $M = N$. In both cases we take

$$r = r^{(n)}, \qquad r' = r^{(n)} - \frac{r^{(0)}}{20\,(n+1)^2}.$$

The estimates (4.36) and (4.37) give us

$$||\sigma^{(n)}|| \leq \text{constant}\left(\frac{(n+1)^2}{r^{(0)}}\right)^{\alpha+d} \cdot \varepsilon^{(n)}, \tag{4.38}$$

$$||\rho_k^{(n)}|| \leq \text{constant}\left(\frac{(n+1)^2}{r^{(0)}}\right)^{2\alpha+2d+1} \cdot \varepsilon^{(n)}. \tag{4.39}$$

To be sure that $\Psi^{(n)}$ is defined on $B\left(r^{(n+1)}\right)$ it is sufficient to subject the norms of ρ_i^n, $i=1, 2, \ldots, d$, to the inequality

$$\sum_{i=1}^{d} \|\rho_i^{(n)}\| < \frac{r^{(0)}}{10\,(n+1)^2}. \tag{4.40}$$

Finally, the explicit formulae (4.16) and (4.24) give us the new error estimate:

$$\max_{i\in\{1,\ldots,d\}} \{\|\delta^{(n+1)}\|, \|\mu_i^{(n+1)}\|\} \leq C\cdot \left(\frac{(n+1)^2}{r^{(0)}}\right)^{2(\alpha+d+1)} \cdot (\varepsilon^{(n)})^2. \tag{4.41}$$

Let us set

$$\varepsilon^{(n+1)} = (\varepsilon^{(n)})^{\frac{3}{2}}.$$

Then our error estimate is reproduced on the $(n+1)$-th step if

$$\varepsilon^{(n)} \leq C^{-2} \left(\frac{r^{(0)}}{(n+1)^2}\right)^{4\,(\alpha+2d+1)}. \tag{4.42}$$

Our choice of N ensures the validity of (4.42) at $n=0$, provided $r^{(0)}$ is chosen sufficiently small. The estimates (4.39) and (4.42) imply (4.40) again if $r^{(0)}$ is sufficiently small. So we can prolong our process to infinity. The estimates (4.38) and (4.39) give us the convergence of the process.

5. CONSTRUCTING THE SERIES (2.1), (2.2)

In order to construct the whole series (2.1), (2.2) we have to find at first (after solving (2.6)) all the functions $\psi_j(x)$ which satisfy the following equations

$$\psi_j(x)^2 = S^0(x) - S^j(x), \qquad j=1, 2, \ldots, d. \tag{5.1}$$

LEMMA 2. – *Let $S^j(x)$, $j=0, 1, \ldots, d$, be taken from the theorem.*

Then the right hand sides in the formulae (5.1) *are the full squares,* i.e. *there exist d unique analytic functions ψ_j, $j=1, 2, \ldots, d$, which satisfy the equations* (5.1) *and have the following convergent series*

$$\psi_j = \sqrt{\omega_j}\, x_j + \sum_{|k|\geq 2} (\psi_j)_k\, x^k, \qquad j=1, 2, \ldots, d, \tag{5.2}$$

in some neighbourhood of the origin.

Proof. – From (3.3) and (4.3) one can easily find that

$$S^0 - S^j = \omega_j x_j^2 + \sum_{|k|\geq 3} (S^0 - S^j)_k x^k, \qquad j = 1, 2, \ldots, d. \tag{5.3}$$

Let us note by $x_{\perp j}$ a point in the $(d-1)$-dimensional space orthogonal to ort_j. According to the Weierstraß preparation theorem for each $j = 1, 2, \ldots, d$, in a neighbourhood of $x_{\perp j} = (0, \ldots, 0)$ there exist analytic functions $f_j(x_{\perp j})$ and $g_j(x_{\perp j})$ such that

$$S^0 - S^j = [x_j^2 + x_j f_j(x_{\perp j}) + g_j(x_{\perp j})] F_j(x), \qquad j = 1, 2, \ldots, d, \tag{5.4}$$

where $F_j(x)$ is an analytic function in some neighbourhood of the origin satisfying the condition $F_j(0, \ldots, 0) \neq 0$.

(From (5.3) one can see that $F_j(0, \ldots, 0) = \omega_j$)

It is easy to see that the equation (2.6) for S^j is equivalent to the following system of equations

$$\begin{cases} \langle \nabla \psi_i, \nabla \psi_j \rangle = \delta_{ij} (\nabla \psi_j)^2, \\ \sum_{i=1}^{d} \psi_i^2 \nabla \psi_i^2 = 2V, \end{cases} \tag{5.5}$$

and it is possible to construct a solution of (5.5) formally in the form (5.2). Indeed, just putting (5.2) into (5.5) and equating the coefficients of each x^k to zero, we obtain the systems of ordinary equations for $(\psi_j)_k$ with not vanishing determinants for $\omega \in \Omega_D$. So we can find recursively coefficients $(\psi_j)_k$ and construct the functions ψ_j as formal series. That means that $S^0 - S^j$ for each $j = 1, 2, \ldots, d$ is a full square in the sense of formal series, and hence the expression in the square brackets of formula (5.4) is a full square in the same sense. This is sufficient for the proof of Lemma 2, because of the analyticity and uniqueness of functions in (5.4). □

After the change of variables (3.4) the equation (2.8) satisfies the conditions of Lemma 1, case (1), $M = 1$, if we choose E_{n1} in the following way:

$$E_{n1} = \sum_{i=1}^{d} \left(n_i + \frac{1}{2} \right) \omega_i . \tag{5.6}$$

According to Lemma 1 there exists an analytic solution which after returning back to coordinates x gives us in some polydisk an analytic solution of (2.8) vanishing at the origin.

Each of the equations (2.9) and (2.11) has the following form

$$\langle \nabla S, \nabla u\rangle + \left(\frac{\Delta S^0}{2} - E_{n1}\right) u = F. \tag{5.7}$$

We look for the solution of (5.7) in the form of the product:

$$u = U\, e^{\mathcal{P}_0}. \tag{5.8}$$

where $\mathcal{P}_0$ is a solution of equation (2.8) for $n = 0$. This means that

$$\langle \nabla S^0, \nabla e^{\mathcal{P}_0}\rangle + \left(\frac{\Delta S^0}{2} - E_{01}\right) e^{\mathcal{P}_0} \equiv 0. \tag{5.9}$$

After putting (5.8) into (5.7) we obtain the following equation for the unknown function U:

$$L_0 \tilde{U} - \langle n, \omega\rangle \tilde{U} = \tilde{F}\, e^{-\tilde{\mathcal{P}}_0}. \tag{5.10}$$

where $L_0 = L_0^0$ is a normal form of the operator $\langle \nabla S^0, \nabla \cdot\rangle$ in coordinates y, "tilde" means the change of variables: $F(x) = \tilde{F}(y)$. Now the left hand side operator is that one of Lemma 1, case (2).

The condition of solvability of the equation (5.10) is the following:

$$(\tilde{F}\, e^{-\tilde{\mathcal{P}}_0})_n = 0, \tag{5.11}$$

$(\tilde{F})_n$ is noting the Taylor coefficient at y^n of the function $\tilde{F}$.

Hence we obtain the following expressions for all the terms of the series (2.1), *i.e.*

$$E_{n2} = -\frac{1}{2}\left([\Delta \tilde{\mathcal{P}}_n + (\nabla \tilde{\mathcal{P}}_n)^2]\right)_0 - \omega^{-\frac{n}{2}} (\tilde{F}_1\, e^{\tilde{\mathcal{P}}_n - \tilde{\mathcal{P}}_0})_n, \tag{5.12}$$

(5.13)
$$E_{nj} = \omega^{-\frac{n}{2}} \left(\left[\frac{\Delta \tilde{u}_{j-1}}{2} - \sum_{l=1}^{j-1} E_{n,l+1}\, \tilde{u}_{n,j-l}\right] e^{-\tilde{\mathcal{P}}_0}\right)_n, \qquad j \geq 2.$$

and find all the functions u_{nj}, $j = 1, 2, \ldots$ in the form (5.8).

6. MAIN THEOREM AND CONCLUDING REMARKS

Results of the paper can be summarized in the following theorem.

THEOREM B. – *Let the potential* V *in Schrödinger equation* (1.1) *be analytic, represented in a neighbourhood of the origin by Taylor series* (3.1) *with positive Diophantine numbers* $\omega_1, \ldots, \omega_d$.

Then for any $n \in \mathbb{N}^d$, $0 \leq |n| \leq n^*$, $N \in \mathbb{N}$, *one can construct the following pair: a number*

$$E_n = \sum_{j=1}^{N} E_{nj}\, \hbar^j,$$

and an analytic function

$$u_n = \exp\left\{-\frac{S^0}{\hbar}\right\} \sum_{j=0}^{N-1} u_{nj}\, \hbar^j.$$

which satisfies the Schrödinger equation (1.1) *up to terms of the order* $\hbar^{N+1} e^{-\frac{s^0}{\hbar}}$ *in some neighbourhood of the origin independent of* $\hbar$. *Here:* $S^0(x)$ *is the positive analytic solution of* (2.6) *with Taylor series* (3.2) (see *Theorem A*), *analytic functions* $u_{nj}(x)$ $(j = 0, 1, \ldots, N-1)$ *and numbers* E_{nj} $(j = 1, 2, \ldots, N)$ *have the form given by formulae* (2.3), (5.2), (5.8) *and* (5.6), (5.12), (5.13).

Remark 6.1. – One can prolong the functions S^j analytically onto a larger domain by the formulae $S^j = \int \sum_{i=1}^{d} p_i^j\, dx_i^j$, $j = 1, 2, \ldots, d$, where for each j the integral is taken along the trajectory of the corresponding Hamiltonian system. Hence one can prolong the functions $\psi_j(x)$, $j = 1, 2, \ldots, d$, and u_{nj}, $j = 0, 1, 2, \ldots$ in the similar way. Thus one can construct sufficient *quasi-modes* in a rather large domain containing the point of a minimum. Then in the problem with many identical wells, situated so that the distances between the points of minimum are finite, one can do the following. Construct *quasi-modes* for each well in such a domain, that the two neighbouring domains intersect. Then multiply those *quasi-modes* on the cutting functions equal to zero beyond the mentioned domains. The approximation for the eigenfunctions of the problem can be taken as a linear combination of these cut-off *quasi-modes*. It is possible then to write down the rigorous splitting formulae following the ideology of [9] for an arbitrary $n \in \mathbb{N}$ in the form as it was obtained in [18]-[20] for $n = 0$. It is important to note that to find the preexponential coefficient in the splitting formula for $|n| > 0$ one has to be sure on the trajectory of the corresponding

Hamiltonian system the corresponding eigenfunction is not equal to zero. Hence one has to investigate the zero-sets of the eigenfunctions.

Remark 6.2. – In order to find the zero-sets of the eigenfunctions one can use as well expansions of the form (2.2). It is more convenient however to construct for this purpose an *ansatz* with Hermite polynomials, namely

$$u_n = \left[e^{\mathcal{P}_n} \prod_{i=1}^{d} H_{n_i} \left(\frac{\psi_i}{\sqrt{\hbar}} \right) + \sum_{j=1}^{\infty} \hbar^j G_j \right] \exp\left\{ -\frac{S^0}{\hbar} \right\}, \tag{6.1}$$

where S^0 and ψ_j, $i \in (1, \ldots, d)$, are the described above functions, $H_{n_i}(t) = (-1)^{n_i} e^{t^2} (e^{-t^2})^{(n_i)}$ are Hermite polynomials which satisfy the following differential equation

$$H''_{n_i}(t) - 2t\, H'_{n_i}(t) + 2\, n_i\, H_{n_i}(t) = 0. \tag{6.2}$$

If we put series (6.1) and (2.1) into the Schrödinger equation (1.1) and equate coefficients at each power of $\hbar$ to zero (taking into account (6.2)) we will obtain problems for G_j quite similar to those described in section 5. Solving them we will construct all the functions G_j, $j = 1, 2, \ldots$ In zero approximation the eigenfunction u_n has the form of an exponent multiplied by a product of Hermite polynomials. Hence in zero approximation we find a set of zeros of the function u_n as a net of intersecting surfaces Σ_i: $\psi_i(x) = t_{ij}$, $i = 1, 2, \ldots, d$, $t_{ij} \in \mathcal{R}_i$, $\mathcal{R}_i$ is a set of roots of $H_{n_i}(t)$. The first term of (6.1) depends on third and forth derivatives of the potential V at the origin. It does not vanish if they are not equal to zero. In this case already in first approximation one can find that Σ_i do not intersect, they have quasi-intersections. A more detailed description of this *ansatz* and some examples will be published elsewhere.

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