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TUNNELING IN MULTIDIMENSIONAL WELLS

T. F. Pankratova
ITMO University, St. Petersburg, Russia
tanpankrat@yandex.ru

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A full asymptotic series for low eigenvalues and eigenfunctions of a stationary Schrödinger operator with a nondegenerate well was constructed in [29]. This allowed us to describe the tunneling effect for a potential with two or more identical wells with sufficient accuracy. The procedure is described in the following discussion. Some formulae are obtained and corresponding problems are discussed.

Keywords: Shrödinger operator, potential, tunneling, eigenvalues and eigenfunctions.

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1. Introduction

Consider the Schrödinger equation:

$$-\frac{h^2}{2}\triangle u + Vu = Eu, \tag{1.1}$$

where $\Delta = \sum_{i=1}^{d} \partial^2/\partial {x_i}^2$ is the Laplace operator, V is a real valued function defined on $\mathbb{R}^d$ having nondegenerate minima (wells) with some mode of symmetry.

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, the 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 connected with some quantum vector $n \in \mathbb{N}^d$), the distance between the groups being of the order h, and the distance between eigenvalues in each group, the splitting, being exponentially small with respect to h.

It is possible to find explicit formulae for the widths of these splittings using semiclassical asymptotics for each well. The problem was considered in different ways by different authors and almost completely solved in the one dimensional case [1–11]. The case $d > 1$ seems much more complicated. There are many results obtained in this area (see [11–20] and the list is far from complete). Still, the picture is not so complete as when $d = 1$. The semiclassical asymptotics of the discrete 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 rigorous asymptotics for the splitting widths in the lowest levels ($n = 0$) were obtained in [18–20] (with the use of a Maslov's canonical operator). Still, there are no effective (as when $d = 1$) splitting asymptotic formulae in terms of the potential for a set of arbitrary levels ($|n| = 1, 2, 3, \ldots$). The possibility of solving this problem in that case was discussed on the Diffraction Day Conference this spring in the talk of A. Anikin and M. Rouleux. These results have not been published yet.

My approach to this problem is different. In order to write down strict asymptotic formulae for splittings in the d-dimensional case, one has to develop methods of [9]. To do so, it is necessary to find a sufficiently accurate semiclassical approximation to eigenstates for a single well in some vicinity of a minimum, independent of h. Such an approximation was constructed in [29]. The formal series on powers of h was obtained. Coefficients in all terms were found in some domain independent of h. 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 an error on the order of $h^{N+1}\exp\left(-S/h\right)$, where S is a nonnegative function defined in [29]. 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 vicinity of a minimum allows one, with the help of *quasi-modes*, to find real eigenfunctions and eigenvalues approximately, with exponentially small errors, smaller than the widths of the splittings. (The program was realized in [9] for $d = 1$.) The constructed series allow us to investigate the set of zeros for the eigenfunctions. The latter is interesting by itself and may be essentially used while finding the splitting asymptotics for $|n| > 1$.

2. Asymptotic expansions for the eigenstates in one well

We look for eigenfunctions u_n and eigenvalues E_n of (1.1) where V is a real valued function defined on $\mathbb{R}^d$ having a nondegenerate minimum at the origin in the form of the following series:

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

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

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

One can find u_{n0} in the following form:

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

where:

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

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

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

$$S^J = \frac{1}{2}\sum_{i=1}^{d} (1 - 2\delta_{ij})\psi_i^2, \quad j = 1, \ldots, d, \quad \delta_{ij} = \begin{cases} 1, & if\ i = j, \\ 0, & if\ i \neq j. \end{cases} \tag{2.5}$$

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

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

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 h to zero. The equation for power 0 is satisfied automatically because of (2.6). The requirement for the coefficient of first degree in h to be equal to zero, gives us the following equation for the function P_n and the number E_{n1}:

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

The analogous requirement for the coefficient of h^2 gives the equation for u_{n1} and E_{n1}:

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

where

$$F_1 = \sum_{i=1}^{d} \frac{n_i(n_i-1)}{2} \psi_i^{n_i-1} (\nabla \psi_i)^2 \prod_{j \neq i} \psi_j^{n_i} + \sum_{i=1}^{d} \frac{n_i}{2} \psi_i^{n_i-1} \Delta \psi_i + \sum_{i=1}^{d} n_i \psi_i^{n_i-1} \left\langle \nabla \psi_i, \nabla P_n \right\rangle \prod_{j \neq i} \psi_j^{n_i}.$$

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

$$\left\langle \nabla S^0, \nabla u_{nj} \right\rangle + \left(\frac{\triangle S^0}{2} - E_{n1} \right) u_{nj} = \\ - \frac{\triangle u_{n,j-1}}{2} + \sum_{l=1}^{j-1} E_{n,l+1} u_{n,j-1} + \psi^n \mathrm{e}^{P_n(x)} E_{n,j+1}. \tag{2.10}$$

In [29], a procedure of constructing solutions for these equations was described and the following theorems were proven.

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 for solutions for equation (2.6) in the form of a power series:

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

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

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

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, $\tilde{v}_k = v_k$ for $|k| = 3$ and $\tilde{v}_k = v_k + \text{terms, depending on } (S^j)_l$, $|l| < |k|$, 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 formally construct these series, we have to impose some additional conditions on the potential V.

Simultaneously, we construct a change of variables:

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

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

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

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

$$\Phi_1^j(y_j) = y_{ij} + \sum_{|k| \geq 2} \left(\Phi_i^j\right)_k y_j^k,. \tag{3.6}$$

In order to find the coefficients $\left(\Phi_i^j\right)_k$, we replace $x_i,\ i = 1, 2, \ldots, d$, in $\langle \nabla S^j,\ \nabla \cdot \rangle$ by $\Phi_1^j(y_j)$ 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:

$$\left(\Phi_i^j\right)_k = \frac{\tilde{S}_{i,j,k}}{\langle k - ort_i\ ,\ I_j \omega \rangle}\ ,\quad j = 0, 1, .., d, \quad |k| \geq 2, \tag{3.7}$$

where:

$$\tilde{S}_{i,j,k} = (k_i + 1) \left(S^j\right)_{k + ort_i} + \text{terms, depending on } \left(\Phi_l^j\right)_m\ ,\quad l = 1, 2, \ldots, d, \quad |m| < |k|\ ,$$

ort_i is an element of a standard basis $\{ort_i\}_1^d$ 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:

(1) we say, that the positive numbers $\omega_1, \omega_2, \ldots, \omega_d$ are *nonresonant-* if they are linearly independent over integers;

(2) 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 $k \in \mathbb{Z}^d$, $k \neq 0$,

$$|\langle k, \omega \rangle| \geq \frac{C}{|k|^{\alpha}}; \tag{3.8}$$

(3) we 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 the vicinity of the origin.*

(1) *If $\in \Omega_{nr}$, 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 vicinity of the origin and satisfies the equation (2.6); and a unique analytic diffeomorphism Φ^0 which transforms the vector field $\langle \nabla S^j,\ \nabla \cdot \rangle$ to the normal form L_0^0 given by (3.5).*

(2) *If $\in \Omega_D$, 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 vicinity of the origin and satisfies the equation (2.6); and a unique analytic, diffeomorphism Φ^j which transforms the vector field $\langle \nabla S^j,\ \nabla\ \rangle$ to the normal form L_0^j given by (3.5).*

The proof of this theorem is published in [29].

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 simplest form for it in suitable variables. Here, we have no given vector fields. We are looking for vector fields which are solutions for 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 a more general situation.

Remark 3.3. One can give the following geometrical interpretation for 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 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 vicinity of that point.

The geometrical aspects of the problem were considered in [27]. In addition to the proof of *Theorem A*, the following lemma was proven.

We denote by B_r a Banach space of analytic functions in $B(r) = y \in \mathbb{C}^d : |y_i| < r$, $i = 1, 2, \ldots, d$ with the norm $\|f\| = \sup_{y\in B(r)} |f(y)|$, by $B_{r,M,n,0}$ the subspace of 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 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 $\{L_n^j\}^{-1}$: $B_{r,M,n,0} \to B_{r',M,n,0}$ which solves the equation $L_n^j = f|_{B(r')}$, $u \in B_{r',M,n,0}$, $f \in B_{r,M,n,0}$, in the following cases:*

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

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

$$\left\|\left\{L_n^0\right\}^{-1}\right\| \leq \frac{c_1}{(r-r')^{d-1}},$$

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

$$\left\|\left\{L_n^0\right\}^{-1}\right\| \leq \frac{c_2}{(r-r')^{\alpha+d}}.$$

4. Constructing the series (2.1), (2.2)

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

$$\psi_j^2(x) = S^0(x) - S^j(x), \qquad j = 1,\ 2,\ \ldots\ , d\ . \tag{4.1}$$

Lemma 2. *Let $S^j(x)$, $j = 0,\ \ldots,\ 1,\ d$, be taken from Theorem A.*

Then, the right hand sides in the formulae (4.1) are the full squares, i.e. there exist d unique analytic functions ψ_j, $j = 1, 2..., d$, which satisfy the equations (4.1) and have the following convergent series:

$$\psi_j = \sqrt{\omega_j}x_j + \sum_{|k|\geq 2} (\psi_j)_k x^k, \qquad j = 1,\ 2,\ \dots\ , d, \tag{4.2}$$

in some vicinity of the origin.

After changing the variables of (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:

$$E_{n1} = \sum_{i=1}^{d} \left(n_i + \frac{1}{2}\right)\omega_i. \tag{4.3}$$

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

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

$$\left\langle \nabla S^0, \nabla u_{n1} \right\rangle + \left(\frac{\triangle S^0}{2} - E_{n1}\right) u_{n1} = F. \tag{4.4}$$

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

$$u = Ue^{P_0}, \tag{4.5}$$

where P_0 is a solution of equation (2.8) for $n = 0$. This means that:

$$\left\langle \nabla S^0, \nabla e^{P_0} \right\rangle + \left(\frac{\triangle S^0}{2} - E_{01}\right) e^{P_0} \equiv 0. \tag{4.6}$$

After putting (4.5) into (4.4) we obtain the following equation for the unknown function U:

$$L_0\tilde{U} - \langle n, \omega\rangle \tilde{U} = \tilde{F}e^{-\tilde{P}_0}, \tag{4.7}$$

where $L_0 = L_0^0$ is the 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 of *Lemma 1*, case (2).

The condition of solvability for equation (4.7) is the following:

$$\left(\tilde{F}e^{-\tilde{P}_0}\right)_n = 0, \tag{4.8}$$

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

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

$$E_{n2} = -\frac{1}{2}\left(\left[\triangle\tilde{P}_n + \left(\nabla\tilde{P}_n\right)^2\right]\right)_0 - \omega^{-\frac{n}{2}}\left(\tilde{F}_1 e^{\tilde{P}_n - \tilde{P}_0}\right)_n, \tag{4.9}$$

$$E_{nj} = \omega^{-\frac{n}{2}}\left(\left[\frac{\triangle\tilde{u}_{j-1}}{2} - \sum_{l=1}^{j-1} E_{n,l+1}\tilde{u}_{n,j-1}\right] e^{-\tilde{P}_0}\right)_n, \qquad j \geq 2; \tag{4.10}$$

and find all the functions u_{nj}, $j = 1, 2, \dots$ in form (4.5).

5. Main theorem and concluding remarks

Results from paper [29] are summarized in the following theorem.

Theorem B. *Let the potential V in Schrödinger equation (1.1) be analytic, represented in a vicinity of the origin by Taylor series (3.1) with positive Diophantine numbers $\omega_1, \omega_2, \dots, \omega_d$.*

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

a number:

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

and an analytic function:

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

which satisfies the Schrödinger equation (1.1) up to terms of the order $h^{N+1}\exp\{-S^0/h\}$ in some vicinity of the origin independent of h. Here: $S^0(x)$ is the positive analytic solution of (2.6) with Taylor series (3.2) (see Theorem A), analytic functions $u_{nj}(x)$ $(j = 0, 1, ..., N-1)$ and numbers $u_{nj}(x)$ $(j = 1, 2, ..., N)$ have the form given by formulae (2.3), (4.2), (4.5) and (4.3), (4.9), (4.10).

Remark 5.1. One can lengthen the functions S^J analytically onto a larger domain by the formulae $S^j = \int \sum_{i=1}^{d} p_i^j dx_i^j$, $j = 1, 2, \dots, d$, where for each j the integral is taken along the trajectory of the corresponding Hamiltonian system. Hence, one can lengthen the functions $\psi_j(x)$, $j = 1, 2, \dots, d$, and u_{nj}, $j = 0, 1, 2, \dots$ in a 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 the minima are finite, one can do the following. Construct *quasi-modes* for each well in such a domain, that the two neighboring 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 then possible to write 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 $n = 0$.

Thus, one can find:

$$\Delta E_n = a_n e^{-b_n/h} \left(1 + O(h)\right),$$

where, in the case $d = 1$, $\quad b_n = \int_{x_1}^{x_2} \sqrt{2V(x)}dx,$

in the case $d \ge 2$, $\quad b_n = \int_{M_1 \check{} M_2} \sqrt{2V(x)}dl,$

the last integral is taken along the extreme line of the functional in the right hand side of the last formula.

It is important to note that to find the pre-exponential coefficient in the splitting formula for $|n| > 0$, one has to be sure that 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. Some examples in a one-dimensional case were considered by my student N. Homchenko and published in [30].

Remark 5.2. In order to find the zero-sets of the eigenfunctions, one can also use expansions of the form (2.2). It is more convenient, however, to construct for this purpose an *ansatz* with Hermite polynomials, namely:

$$u_n = \left[e^{P_n} \prod_{i=1}^{d} H_{n_i} \left(\frac{\psi_i}{\sqrt{h}} \right) + \sum_{j=1}^{\infty} h^j G_j \right] \exp \left\{ -\frac{S^0}{h} \right\}, \tag{5.1}$$

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

$$H''_{n_i}(t) - 2tH'_{n_i}(t) + 2n_i H_{n_i}(t) = 0. \tag{5.2}$$

If we put series (5.1) and (2.1) into the Schrödinger equation (1.1) and equate coefficients at each power of h to zero (taking into account (5.2)), we will obtain problems for G_j quite similar to those described in Section 4. Solving them, we will construct all the functions G_j. In zero approximation the eigenfunction u_n has the form of an exponent multiplied by a product of Hermite polynomials. Hence, in the zero approximation, we find a set of zeros of the function u_n as a net of intersecting surfaces $\Sigma_i : \psi_i(x) = t_{ij}$, $i = 1, 2, \ldots, d$, $t_{ij} \in R_i$, R_i is a set of roots of $H_{n_i}(t)$. The first term of (5.1) depends on third and fourth derivatives of the potential V at the origin. It does not vanish if they are not equal to zero. In this case, one can already find in the first approximation, that Σ_i do not intersect. They have quasi-intersections. A more detailed description of this *ansatz* and some examples were published in [31] and [32].

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