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N wells at a circle. Splitting of lower eigenvalues

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A stationary Schrödinger operator on $\mathbb{R}^2$ with a potential V having N nondegenerate minima which divide a circle of radius r_0 into N equal parts is considered. Some sufficient asymptotic formulae for lower energy levels are obtained in a simple example. The ideology of our research is based on an abstract theorem connecting modes and quasi-modes of some self-adjoint operator A and some more detailed investigation of low energy levels in one well (in $\mathbb{R}^d$).

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1. Introduction. Modes and quasi-modes

We use terms modes and quasi-modes following V. I. Arnold [1]. An eigenvalue and eigenvector of some operator A, i.e. a pair (λ, u) which satisfies equation $Au = \lambda u$ exactly, is called a mode. Some value and vector which satisfy this equation approximately with some error of order ε is called a quasi-mode. More precisely, the result is as follows:

Let A be a self-adjoint operator in a Hilbert space H, λ_0 – a real value, orthonormal vectors $u_1, u_2, ..., u_N \in D(A)$, Q is a positive constant, $\varepsilon = \max\limits_{1 \le i \le N} \|(A - \lambda_0)\, u_i\|$, $0 < 4\sqrt{3}N\varepsilon < Q$, $\lambda_1, ..., \lambda_N$ are the eigenvalues of the matrix M with the inputs $\{M_{ik}\} = \{\langle Au_i, u_k\rangle\}$ ($\langle\cdot,\cdot\rangle$ means a scalar product in H), every eigenvalue is counted according to its multiplicity.

Theorem 1. *Suppose the interval* $I = [\lambda_0 - Q, \lambda_0 + Q]$ *contains at most* N *eigenvalues of* A*. Then, the interval* $I_1 = \left[\lambda_0 - Q + 4\sqrt{3}N\varepsilon, \lambda_0 + Q - 4\sqrt{3}N\varepsilon\right]$ *contains exactly* N *eigenvalues of* A*. There exist constants* p *and* q *such that if* $0 < \varepsilon < p$ *then, any interval* $\delta_j = \left[\lambda_j - q\varepsilon^2, \lambda_j + q\varepsilon^2\right]$ *is included in* I_1 *and contains an eigenvalue of* A*. Any connected component of the set* $\bigcup\limits_{j=1}^{N} \delta_j$ *contains exactly as many eigenvalues of* A *as there are intervals* δ_j *forming it.*

Theorem 1 allows us to describe eigenvectors and eigenvalues of A based on the knowledge only of its quasi-modes. If δ_j does not intersect with δ_{j+1}, the distance between their middle points gives us a good approximation of the distance between the two nearest eigenvalues. The first proposition of Theorem 1 guaranties the absence of additional eigenvalue of A in our interval.

2. A self-adjoint Schrödinger operator on $\mathbb{R}^d$

Let us consider the Schrödinger equation:

$$-\frac{h^2}{2}\Delta u + Vu = Eu, \tag{1}$$

where $\Delta = \sum\limits_{i=1}^{d} \dfrac{\partial^2}{\partial_i^2}$ is the Laplace operator, V is a real valued function defined on $\mathbb{R}^d$ having nondegenerate minima (wells) with some kind of symmetry, h (small parameter) is the Planck constant (in special system of units). Let A be the corresponding Schrödinger operator defined by the left hand side of equation (1) in $L_2(\mathbb{R}^d)$.

If V in (1) 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 operator A is organized in the following way. There is a set of finite groups of eigenvalues (each of them is related to 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 semi-classical asymptotics for each well. The problem was considered in different ways by different authors and almost completely solved in one dimensional case [1–8]. The case $d > 1$ is much more complicated. There are many results obtained in this area (see [9–17] and the list is far from exhaustive). The semiclassical asymptotics of the discrete spectrum and strict estimates of the splittings are described in [9] 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 were obtained in [10] (with the use of Maslov's canonical operator). The possibility to solve this problem in that case was discussed during the Diffraction Day Conference 2014 in the talk of A. Anikin and M. Rouleux [12].

In the present work, in order to write down strict asymptotic formulae for splittings in two-dimensional case, one has to use Theorem 1. 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 [11, 13]. The formal series on powers of h were 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 m-th term the remaining sums satisfy the equation (1) with an error of the order of $h^{m+1}\exp(-S/h)$, where S is a nonnegative function defined in [11]. The possibility to take m as large as we like and exponential decreasing of all terms beyond some vicinity of a minimum allows one to construct sufficient *quasi-modes*. Each *quasi-mode* has to be constructed from semiclassical approximations of lower eigenfunctions in the region of the bottom of each well vanishing beyond it.

In this work, a simple example is considered. Here, the circle containing N minima of V is f line of minimum of the corresponding functional b and it is easy to find b in a plain form.

3. An example. N wells at a circle

Let $d = 2$. Let V in equation (1) in polar coordinates be of the following form:

$$V = \frac{\omega_1^2}{2}(r - r_0)^2 + \frac{\omega_2^2}{2}\sin^2\frac{N\phi}{2}, \tag{2}$$

ω_1, ω_2 are some positive Diophantine numbers. (This means that there exist positive numbers α and β such that for any $k \in \mathbb{Z}^2$, $k \neq 0$, $|\langle k, \omega\rangle| \geq \dfrac{\beta}{|k|^\alpha}$).

It is easy to see that the points $M_j\left(r_0; \dfrac{2\pi j}{N}\right)$, $j = 0, 1, ..., N-1$, are nondegenerate minima of V, $M_j \in \Gamma$, Γ is a circle $r = r_0$ and

$$V(r, \phi) = V\left(r; \phi + \frac{2\pi j}{N}\right). \tag{3}$$

We put a Cartesian system of coordinates $(x_j; y_j)$ in the vicinity of the bottom of each well in such a way that $M_j = M_j(0; 0)$ in this coordinates, axis x_j is tangential to a circle Γ at the point M_j and y_j is normal to it. One can find the following Taylor series for V:

$$V(X_j) = \frac{1}{2}\left(\hat{\omega}_1^2 x_j^2 + \hat{\omega}_2^2 y_j^2\right) + \sum_{|k|\geq 3} v_k X_j^k,$$

$$X_j = (x_j; y_j), \quad k = (k_1; k_2), \quad X_j^k = x_j^{k_1} y_j^{k_2}, \quad |k| = k_1 + k_2, \quad \hat{\omega}_i > 0, \quad i = 1, 2,$$

in a vicinity of M_j. The form of this series does not depend on j because of equality (3).

In order to use Theorem 1, let us find semiclassical approximations $\left(\hat{u}_n, \hat{E}_n\right)$ for some first quantum vectors $n = (n_1, n_2)$, $n_1 = 0, 1, ...$; $n_2 = 0, 1, ...$; in each domain $D_j = \{|x_j| \leq \gamma, |y_j| \leq \hat{\gamma}\}$. They are the same for all D_j, $j = 0, 1, ...N-1$. Let us take numbers γ and $\hat{\gamma}$ such that two neighboring domains D_j and D_{j+1} intersect. Let domain $G_{j,j+1} = D_j \bigcap D_{j+1}$ be such an intersection. Let the point $\hat{M}_j = \hat{M}_j\left(r_0; \dfrac{\pi(2j+1)}{N}\right) \in G_{j,j+1}$, $j = 0, 1, ..., N-1$. Then, we multiply $\hat{u}_n$ by cutting functions $\chi^{[j]} = \chi^{[j]}(x_j, y_j) = \chi_1^{[j]}(x_j)\,\chi_2^{[j]}(y_j)$, where

$\chi_1^{[j]}(x_j)$ and $\chi_2^{[j]}(y_j)$ are smooth cutting functions, i.e.

$$\chi_1^j(x_j) = \begin{cases} 1, & |x_j| \le \gamma, \\ 0, & |x_j| \ge \gamma + \varepsilon_1, \end{cases} \qquad \chi_2^j(y_j) = \begin{cases} 1, & |y_j| \le \hat{\gamma}, \\ 0, & |y_j| \ge \hat{\gamma} + \varepsilon_2, \end{cases} \qquad \hat{u}_n \chi^{[j]} = \hat{u}_n^{[j]}.$$

Function $\hat{u}_n^{[j]}$ is equal to zero beyond rectangular $\{|x_j| \ge \gamma + \varepsilon_1, |y_j| \ge \hat{\gamma} + \varepsilon_2\}$. We construct N quasi-modes $\tilde{u}_{n,k}$, $k = 1, ..., N$, as a linear combination of cut-off functions $\hat{u}_n^j$, i.e. $\tilde{u}_{n,k} = \sum\limits_{j=1}^{N} \alpha_{j,k} \hat{u}_n^{[j]}$, $k = 1, ..., N$. We find numbers $\alpha_{j,k}$ in order to orthonormalize the system $\{\tilde{u}_{n,k}\}_{k=1}^{N}$. Now, we can use Theorem 1 in a way similar to one presented in [8].

We find that for our example with N wells (eq. (2)) for each quantum vector N eigenvalues E_n^k, $k = 1, ..., N$, of operator A has the following form:

$$E_n^k = \hat{E}_n + \mu_k^{[n]} + O\left(\varepsilon^2\right),$$

where:

$$\hat{E}_n = \sum_{j=1}^{m} E_{n,j} h^j; \quad E_{n,1} = \left(n_1 + \frac{1}{2}\right)\hat{\omega}_1 + \left(n_2 + \frac{1}{2}\right)\hat{\omega}_2,$$

$$\mu_k^{[n]} = a \cdot \exp\left(-h^{-1} b\right) \cdot \cos\frac{\pi k}{N+1}, \quad k = 1, ..., N, \quad \mu_k^{[n]} = O(\varepsilon), \quad b = \int\limits_{M_{k-1}M_k} \sqrt{2V} dS,$$

$M_{k-1}M_k$ is a line of minimum of functional b. In our case it is a part of the circle Γ. At this circle, $\sqrt{2V} = \omega_2 \sin\frac{N\phi}{2}$, $dS = r_0 d\phi$. Hence, $b = \frac{4}{N} r_0 \omega_2$.

Now, we can write down the splitting formula for lower eigenvalues of operator A:

$$\Delta E_n^k = E_n^{k+1} - E_n^k = d_k \exp\left(-\frac{b}{h}\right)(1 + O(h)), \quad k = 1, ..., N.$$

One can regard this example as a simple model for some possibly more complicated situation.

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