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Approximation of point perturbations on finite set of Laplace-Beltrami operator on Riemannian manifold

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Abstract. The work is devoted to the substantiation of zero-range potentials in case of non-trivial geometry. We bind two approaches to point perturbations: restriction-extension and approximation by family of Schrödinger operators with regular potentials.

1. Motivation
Kronig and Penney introduced zero-range potentials in 1931 to describe the motion of non-relativistic electron in a rigid crystal lattice [3], and since then point perturbations are often used in mesoscopic physics to obtain exact solvable models. In the paper [6] Tomas showed the necessity of approximation of zero-range potentials by short-distance potentials. To prove the correspondence of mathematical model to real system one should know the approximation by regular potentials. For Euclidean spaces this question is well elaborated (see [1]).

In the year 1991 Mackay and Terrones introduced conception of periodic graphene layers with negative Gaussian curvature. They showed that this structures are energetically stable, and therefore are producible. ([5], [4])

Due to the appearance of such materials it is necessary to prove possibility and study properties of the approximation of point potentials on Riemannian manifolds.

2. Target setting
Let $X$ be a three dimensional compact Riemannian manifold of bounded geometry. The Hamiltonian of a free charged particle on $X$ is the Laplace-Beltrami operator

\[ H^0 = -\Delta_{LB} \]

where $\text{dom}(H^0) = C_0^\infty(X)$. Formally the perturbation of this operator by zero-range potentials, supported at distinct points $\{q_k\}_{k=1}^n \in X$, is given by

\[ H_q = -\Delta_{LB} + \sum_{k=1}^n a_k \delta(\cdot - q_k) \]

The strict mathematical sense of such perturbation can be adjusted by theory of self-adjoint extensions of symmetric operators or using approximation by Hamiltonians with regular
potentials. We will bind these two approaches. First we construct Hamiltonian with point perturbation \( H_A \) using theory of self-adjoint extensions, then we provide sequence of Hamiltonians with regular potentials which tends in norm resolvent sense to \( H_A \).

3. Construction of point perturbations using theory of self-adjoint extensions

Consider a restriction \( S_q \) of \( H^0 \) onto functions which are equal to zero in the vicinity of perturbation centers. Self-adjoint extensions of \( S_q \) are called point perturbations of \( H^0 \).

The operator \( S_q \) has deficiency indices \((n, n)\). To construct resolvent of its self-adjoint extensions we use Krein’s theory (see \([2]\))

The Green function of Laplace-Beltrami operator on a three dimensional manifold can be decomposed in the following way:

\[
G^0(x, y; z) = G^0_{\text{ren}}(x, y; z) + \frac{1}{\rho(x, y)}
\]  

(3)

where \( G^0_{\text{ren}}(x, y; z) \) is a continuous part of the Green’s function, and \( \rho(x, y) \) is the geodesic distance between points \( x \) and \( y \).

A Krein’s \( Q \)-function \( Q \) can be defined by their matrix elements as follows: \( Q(z): \mathbb{C}^n \rightarrow \mathbb{C}^n \),

\[
Q_{ij}(z) = \begin{cases} 
G^0_{\text{ren}}(q_i, q_i; z), & i = j \\
G^0(q_i, q_j; z), & i \neq j 
\end{cases}
\]  

(4)

By the Krein’s theory the extension is characterized by a self-adjoint linear operator \( A: \mathbb{C}^n \rightarrow \mathbb{C}^n \) as a parameter. And the resolvent of perturbed operator has the form

\[
R_A(z) = (H^0 - z)^{-1} - \sum_{i=1}^{n} \sum_{j=1}^{n} \left\{ [Q(z) - A]^{-1} \right\}_{ij} G^0(\cdot, q_i; z) < G^0(q_j, \cdot; z)\cdot >
\]  

(5)

4. Construction of approximation

Consider the following one-parametric family of Hamiltonians with regular potentials

\[
H_\varepsilon = -\Delta_{LB} + \frac{1}{\varepsilon^2} \sum_{i=1}^{n} \lambda_i(\varepsilon) V_i(\theta_{q_i}^{-1}(\varepsilon, \cdot))
\]  

(6)

where \( \lambda_i(\varepsilon) \) are real-valued analytic functions, \( \lambda_i(0) = 1 \), \( V_i \) are regular potentials which are greater than zero on their supports, and \( \theta_{q_i}^{-1} \) is the inverse dilation with centers at points \( q_i \). We look for conditions under which this family of Hamiltonians converges in some sense to point perturbation constructed using restriction-extension method.

To formulate the main result of the work we need to introduce some mathematical objects originating from non-trivial geometry. First of all we consider Jacobian of map \( \theta_{q_i}(\varepsilon, \cdot): X \rightarrow X \). We can introduce special function which indicates the deviation of this Jacobian in Riemannian case from Euclidean case

\[
J_i(y) = \lim_{\varepsilon \rightarrow 0} \frac{\text{Jac}(\theta_{q_i}(\varepsilon, y))}{\varepsilon^3}
\]  

(7)

We assume that \( 0 < c_i < J_i(y) < C_i < +\infty \) on the support of \( V_i \). Such assumptions restrict the class of possible manifolds, but it can be proved that nearly all manifolds interesting for applications satisfy these conditions for sufficiently small supports of regular potentials \( V_i \).

Next object appears, because the cosine theorem is not true for triangle consisted of geodesics:

\[
\rho(\theta_{q_i}(\varepsilon, \cdot), \theta_{q_i}(\varepsilon, y)) = c \omega_1(x, y; q_i) + o(\varepsilon)
\]

\[
\omega_1(x, y; q_i) = \sqrt{\rho^2(x, q) + \rho^2(y, q) - 2 \cos(\alpha) \rho(x, q) \rho(y, q)}
\]
where $\alpha$ is the angle between tangent vectors to geodesics $\dot{x}q$ and $\dot{y}q$. Assume that
\[ \int_{X \times X} \frac{1}{\omega_1(x,y; q_i)} dx dy < +\infty. \]

The main result of our work can be derived from spectral analysis of operator $B_0$ with the matrix integral kernel of the following form
\[ B_{0,ij} = \begin{cases} \sqrt{V_i(x)V_j(y)J_i(x)J_j(y)} & i = j \\ 0 & i \neq j \end{cases} \] (8)

**Theorem 4.1** There are two main cases:

(i) If $-1$ is not an eigenvalue of operator $B_0$ then $H_\epsilon \to H_0$ in the norm resolvent sense.

(ii) If $-1$ is a simple eigenvalue of $B_0$ and $\phi = (\phi_1, \ldots, \phi_n)^T$ is a normalized eigenfunction ($<\phi_i|\phi_i> = 1$) then $H_\epsilon \to H_\Lambda$ in the norm resolvent sense and $\Lambda$ is a diagonal matrix such that
\[ A_{ii} = \frac{\lambda'_i(0)}{<\sqrt{J_i}V_i|\phi_i>} \] (9)

5. Conclusion

This work is devoted to basement of zero-range potentials in case of complicated geometry. Further investigations may touch point perturbations on two dimensional Riemannian manifolds, because many promising structures can be represented as such manifolds. It is interesting for nanotechnology to study point perturbations on $S^2$ and on infinite cylinders, because they correspond to fullerenes and nanotubes accordingly. In the scope of our interest are also perturbations with a curve-shaped support on two dimensional manifolds. Authors thank Prof. I. Popov and D. Ivanov for useful discussions.

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