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Higher-Order Spectral Shift Functions and Associated Trace Formulas for One-Dimensional Schrödinger Operators

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Abstract. Spectral shift functions (SSFs) provide a powerful framework for understanding how the spectrum of a self-adjoint operator changes under perturbation, and they play a central role in trace formulas that generalize the classical results of Krein and Koplienko. While higher-order SSFs have been extensively developed in abstract settings—particularly under Schatten class assumptions or within noncommutative frameworks with τ-compact resolvents—their explicit computation remains challenging, especially for differential operators arising in quantum mechanics. In this paper, we define and compute the SSF of order k for a one-dimensional Schrödinger operator perturbed by a constant potential, and rigorously verify the associated trace formula. Our approach, grounded in classical Hilbert–Schmidt theory and Fourier analysis, bypasses abstract machinery while capturing physically meaningful scenarios. These results also serve as a foundation for future work on more singular perturbations, such as delta and square-well potentials.

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1. INTRODUCTION

Perturbation theory plays a central role in mathematical physics, particularly in quantum mechanics, where Hamiltonians [1] often model systems subject to external forces or fields. Given a self-adjoint operator H_0 and a perturbation V, the primary object of interest is $H = H_0 + V$. The fundamental question is how the spectral properties of H differ from those of H_0.

One of the most effective tools to study this problem is the spectral shift function (SSF), introduced heuristically by Lifshits in the 1940s and rigorously by Krein in 1953. The SSF quantifies the change in the spectral measure under perturbations and appears naturally in trace formulas. Krein's trace formula has since been extended to higher-order cases in several directions, often involving Taylor-like remainders for operator functions [2, 3].

Let H_0 be an unbounded self-adjoint operator, V a bounded self-adjoint operator on a separable Hilbert space $\mathscr{H}$, and f a sufficiently smooth function, with $f(H_0)$ and $f(H_0+V)$ be defined via the functional calculus. Consider the remainder of the Taylor approximation

$$R_{n,H_0,V}(f) := f(H_0+V) - \sum_{k=0}^{n-1} \frac{1}{k!} \frac{d^k}{dt^k}\Big|_{t=0} f(H_0+tV),$$

where $n \in \mathbb{N}$ and the Gâteaux derivatives $\frac{d^k}{dt^k}\Big|_{t=0} f(H_0+tV)$ are evaluated in the uniform operator topology. If a perturbation $V = V^*$ is in the Schatten-von Neumann ideals of compact operators $\mathscr{S}^n$, then the following trace formula holds

$$\mathrm{Tr}\big(R_{n,H_0,V}(f)\big) = \int_{\mathbb{R}} f^{(n)}(t)\eta_n(t)\,dt, \tag{1}$$

where $\eta_n = \eta_{n,H_0,V}$ is a real valued $\mathscr{L}^1$-function depending only on H_0 and V. The formula (1), for $n = 1$, is the Krein's trace formula [4]. The cases $n = 2$ and $n \geq 3$ were established by L. S. Koplienko in 1984 [5] and by D. Potapov, A. Skripka, and F. Sukochev in 2013 [2], respectively.

If the perturbation V is not compact, then $\mathrm{Tr}\big(R_{n,H_0,V}(f)\big)$ may be undefined, and one must impose additional conditions on H_0 and f to ensure that $R_{n,H_0,V}(f)$ belongs to the trace class. Such perturbations often arise in the study of differential operators, as these are typically multiplication operators on $\mathbb{R}^d$, which are not compact. In this case, the condition $V \in \mathscr{S}^n$ is typically replaced with assumptions on the resolvent of the unperturbed operator H_0. For example, if the resolvent of H_0 is compact and $f \in C_c^3(\mathbb{R})$, then formula (1) holds for $n = 1$ (See [6] (Theorem 2.5)).

In recent years, the analysis of higher-order SSFs in such settings has advanced considerably, especially in noncommutative contexts involving semifinite von Neumann algebras. For instance, in [7, 8], the authors establish trace formulas for operators with τ-compact resolvents in a semifinite von Neumann algebra setting, assuming $f \in C_c^{n+1}(\mathbb{R})$, or more generally $f \in C_c^n(\mathbb{R})$ with $f^{(n)}$ bounded.

This paper contributes to the theory by computing higher-order SSFs in the case of the Laplacian perturbed by a constant potential. Our approach, based on classical Hilbert–Schmidt perturbation theory and Fourier analysis, avoids reliance on abstract frameworks. While purely computational, our results offer a rigorous treatment of explicit examples relevant to quantum systems and lay the groundwork for studying more singular potentials, such as delta and square-well interactions.

2. COMPUTATIONAL METHODS

This section outlines the mathematical framework used to explicitly compute higher-order spectral shift functions (SSFs) and verify the associated trace formulas. We focus on a concrete, analytically tractable example in quantum mechanics: the one-dimensional Schrödinger operator perturbed by a constant potential. The aim is to provide explicit formulas for SSFs and trace expressions that are both rigorous and physically meaningful.

Let $\mathscr{H} = L^2([0,\pi])$ and consider the unperturbed operator H_0 defined on the domain

$$\mathscr{D} = \left\{ \begin{array}{r} u \in L^2([0,\pi]) : u' \text{ is absolutely continuous,} \\ u'' \in L^2([0,\pi]),\ u(0) = u(\pi) = 0 \end{array} \right\}$$

by the rule $H_0 u = -u''$. This is the standard Dirichlet Laplacian, whose eigenvalues are $\lambda_n = n^2$ with normalized eigenfunctions $\phi_n(x) = \sqrt{\frac{2}{\pi}}\sin(nx)$.

We consider a perturbation V given by a constant potential: $V(x) = c \in \mathbb{R}$. Then the perturbed operator $H = H_0 + V$ has eigenvalues $\mu_n = n^2 + c$ and shares the same eigenfunctions as H_0.

Since both H_0 and H have compact resolvents, spectral shift functions can be defined using finite-rank spectral projections. For any compact set $\delta \subset \mathbb{R}$, the spectral projection $E_{H+tV}(\delta)$ has finite rank, and its trace equals the number of eigenvalues of $H + tV$ in δ.

Let $a < 1$ and assume $0 < c < 3$. Define the first-order spectral shift function by

$$\eta_1(\lambda) := \operatorname{Tr}\left(E_{H_0}((a,\lambda]) - E_H((a,\lambda])\right).$$

Then, for each $n \in \mathbb{N}$:

$$\eta_1(\lambda) = \begin{cases} 0 & \text{if } a < \lambda < 1, \\ 1 & \text{if } n^2 \le \lambda < n^2 + c, \\ 0 & \text{if } n^2 + c \le \lambda < (n+1)^2. \end{cases} \tag{2}$$

Clearly, η_1 is locally integrable on $\mathbb{R}$.

Now define, for a subset $A \subset \mathbb{R}$,

$$\delta_{n^2}(A) := \begin{cases} 1 & \text{if } n^2 \in A, \\ 0 & \text{otherwise,} \end{cases}$$

and for each $k \in \mathbb{N}$, define a measure:

$$\mu_k(A) := \sum_{n=1}^{\infty} \frac{c^k}{k!}\, \delta_{n^2}(A),$$

which is locally finite. Then, for $a < 1$ and $0 < c < 3$:

$$\mu_k((a,\lambda]) = \begin{cases} 0 & \text{if } a < \lambda < 1, \\ \frac{nc^k}{k!} & \text{if } n^2 \le \lambda < n^2 + c, \\ \frac{nc^k}{k!} & \text{if } n^2 + c \le \lambda < (n+1)^2. \end{cases} \tag{3}$$

For $k \ge 2$, we define the k-th order SSF recursively as:

$$\eta_k(\lambda) := \mu_{k-1}((a,\lambda]) - \int_a^{\lambda} \eta_{k-1}(t)\, dt. \tag{4}$$

3. MAIN SECTION

Let H be a self-adjoint operator in a Hilbert space $\mathscr{H}$, and let $V = V^* \in \mathscr{B}(\mathscr{H})$. Given a function $f : \mathbb{R} \to \mathbb{C}$, the Gâteaux derivative of the mapping $H \mapsto f(H)$ in the direction V is defined by:

$$\left.\frac{d}{ds}\right|_{s=0} f(H + sV) := \lim_{s \to 0} \frac{f(H+sV) - f(H)}{s},$$

provided the limit exists in the operator norm.

Using the spectral theorem and Taylor expansion, we have the k-th order remainder:

$$\operatorname{Tr}(R_{k,H_0,V}(f)) = \sum_{n=1}^{\infty} \left(f(n^2 + c) - \sum_{j=0}^{k-1} \frac{c^j}{j!} f^{(j)}(n^2) \right). \tag{5}$$

We now compute η_k for small values of k. From (4), using previously defined η_1 and μ_1:

$$\begin{aligned} \eta_2(\lambda) &= \mu_1((a,\lambda]) - \int_a^{\lambda} \eta_1(t)\, dt \\ &= \begin{cases} 0 & \text{if } a < \lambda < 1, \\ -\lambda + c + n^2 & \text{if } n^2 \le \lambda < n^2 + c, \\ 0 & \text{if } n^2 + c \le \lambda < (n+1)^2, \end{cases} \end{aligned}$$

and similarly:

$$\eta_3(\lambda) = \mu_2((a,\lambda]) - \int_a^\lambda \eta_2(t)\,dt$$
$$= \begin{cases} 0 & \text{if } a < \lambda < 1, \\ \dfrac{\lambda^2}{2} - (c+n^2)\lambda + cn^2 + \dfrac{c^2}{2} + \dfrac{n^4}{2} & \text{if } n^2 \le \lambda < n \\ 0 & \text{if } n^2 + c \le \lambda \end{cases}$$

These satisfy: $\eta_k' = -\eta_{k-1}$, $\eta_k(n^2) = \dfrac{c^{k-1}}{(k-1)!}$, and $\eta_k(n^2+c) = 0$.

Now, using these properties:

$$\int_{\mathbb{R}} f^{(k)}(\lambda)\eta_k(\lambda)\,d\lambda = \sum_{n=1}^{\infty} \int_{n^2}^{n^2+c} f^{(k)}(\lambda)\eta_k(\lambda)\,d\lambda$$
$$= \sum_{n=1}^{\infty} \left(f(n^2+c) - \sum_{j=0}^{k-1} \frac{c^j}{j!} f^{(j)}(n^2) \right), \tag{6}$$

which matches the earlier expression (5), completing the proof of the trace formula (1) for our concrete example.

4. EXAMPLE: LAPLACIAN WITH CONSTANT POTENTIAL

We now illustrate the explicit computation of the first-, second-, and third-order spectral shift functions in the case of the one-dimensional Laplacian on $[0,\pi]$ with Dirichlet boundary conditions, perturbed by a constant potential c. The unperturbed operator H_0 has eigenvalues $\lambda_n^{(0)} = n^2$, while the perturbed operator $H = H_0 + c$ has eigenvalues $\lambda_n = n^2 + c$. For $0 < c < 3$, the trace formulas yield piecewise constant, linear, and quadratic spectral shift functions η_1, η_2, and η_3, respectively.

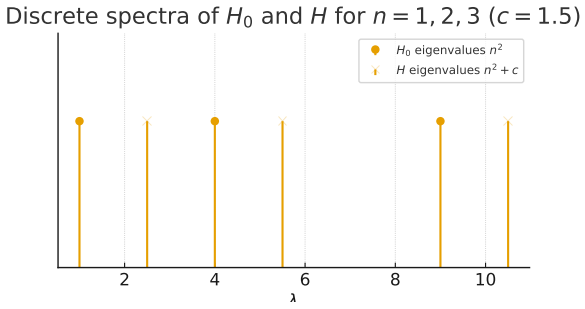

FIGURE 1: Discrete spectra of H_0 (eigenvalues n^2) and H (eigenvalues $n^2 + c$) with $c = 1.5$. Each eigenvalues of H_0 is shifted to the right by the constant c, producing the spectrum of H.

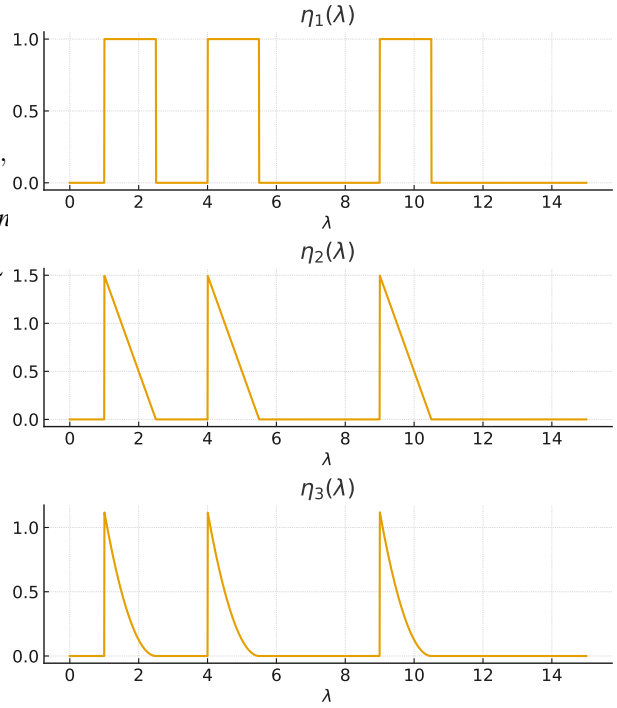

FIGURE 2: First-, second-, and third-order spectral shift functions η_1, η_2, and η_3 corresponding to the perturbation by a constant potential $c = 1.5$. The functions are piece-wise constant, linear, and quadratic, respectively, reflecting the analytic structure predicted by the trace formulas.

This example demonstrates how higher-order spectral shift functions capture progressively finer information about the spectral perturbation. In particular, η_1 counts eigenvalue shifts, η_2 provides a linear correction, and η_3 reflects quadratic dependence on λ.

5. RESULTS AND DISCUSSION

The computations presented in the previous section verify that higher-order spectral shift functions (SSFs) η_k can be explicitly computed for a simple, yet physically relevant, class of perturbations—constant potentials on a bounded interval with Dirichlet boundary conditions. These functions satisfy the recursive relations $\eta_k' = -\eta_{k-1}$ and boundary values consistent with the trace formula of order k.

Equation (6) confirms the trace identity (1) for all $k \in \mathbb{N}$ and for compactly supported smooth functions f, thereby validating the correctness of our definition of η_k. The piecewise nature of η_k illustrates a striking feature: while the spectral shift measure becomes more regular as k increases (eventually becoming absolutely continuous), the

support of η_k remains confined to the intervals $[n^2, n^2 + c)$, making them computationally accessible.

This study also confirms that the assumption of a compact resolvent (as satisfied by $H_0 = -\Delta$ on a bounded interval) suffices to render all operators $R_{k,H_0,V}(f)$ trace-class for $f \in C_c^k(\mathbb{R})$. Our results thus bridge the gap between abstract noncommutative settings and concrete examples arising in quantum mechanics. Moreover, the recursive structure of η_k offers an efficient computational method for constructing higher-order SSFs without recourse to noncommutative geometry or perturbation determinants.

These results not only support existing trace formulas but also pave the way for investigating spectral shift functions in more singular scenarios, such as delta and square-well potentials—where analytic techniques become substantially more involved.

6. CONCLUSION

In this paper, we presented an explicit computation of higher-order spectral shift functions and the corresponding trace formulas in the context of one-dimensional Schrödinger operators perturbed by constant potentials. By working in the concrete setting of the Laplacian on a bounded interval, we avoided the technical complications of abstract frameworks while still verifying deep spectral trace identities.

Our approach reveals how the spectral shift functions η_k emerge naturally from the analysis of the Taylor remainder of operator functions and shows that such functions are not only well-defined but also computable in closed form under suitable spectral assumptions. In particular, we demonstrated that for operators with compact resolvents and constant perturbations, the trace of the k-th order remainder $R_k(f)$ can be recovered via an integral involving η_k and $f^{(k)}$.

The techniques employed here set the foundation for further study of more singular perturbations, such as delta interactions or square-well potentials, and potentially offer insights into the spectral flow and scattering theory (see, [9]) in more general settings. Future work will focus on extending these methods to discontinuous or distributional potentials, and on analyzing the regularity and asymptotics of η_k in such regimes.

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