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On-diagonal singularities of the Green functions for Schrödinger operators

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We investigate the behavior of the Green functions of Schrödinger operators near the diagonal. The only nontrivial cases, where the on-diagonal singularities are nonzero and do not depend on the spectral parameter, are two and three dimensions. In the case of two dimensions we show that the singularity is independent of both the scalar and the gauge potentials. In dimension three, we obtain conditions for preserving the singularity under perturbations by nonregular potentials. Some examples illustrating dependence of the singularity on general scalar and gauge potentials are presented. © *2005 American Institute of Physics.*
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I. INTRODUCTION

Singularities of the Green functions of quantum-mechanical operators play a crucial role in many branches of theoretical and mathematical physics, from which one should mention first the renormalization procedure of the quantum field theory.[1,2] From the point of view of the high-derivative quantum gravity, the corresponding problem was considered, e.g., in Ref. 3. In particular, in the case of nonminimal coupling of quantum matter to the gravitational background with conical singularities, an operator of the form $H=-\Delta+V$ arises on a Riemannian manifold X. Here Δ is the Laplace-Beltrami operator on X and V represents the nonminimal coupling term $\xi\mathcal{R}$ with the Ricci scalar $\mathcal{R}$. The scalar curvature possesses a distributional behavior at conical singularities,[4] $\mathcal{R}=\mathcal{R}_{\text{reg}}+4\pi(1-\alpha)\delta_M$, where δ_M is a Dirac δ-like potential supported by a submanifold $M\subset X$ and $2\pi(1-\alpha)$ is the angle deficit. As a result, an operator

$$H_M = -\Delta + U + a\delta_M \tag{1.1}$$

arises where $U=\xi\mathcal{R}_{\text{reg}}$ and the coupling constant $a=4\pi\xi(1-\alpha)$ characterizes the interaction with the background field concentrated on M. Operators of such form appear in the investigation of scalar fields with nonminimal coupling on the cosmic string background, in the Euclidean approach to the black hole thermodynamics, in the study of the particle scattering at the Planck scale (see Ref. 4 and references therein). Moreover, in the context of the scattering theory, the potential U can have singularity (e.g., of the Coulomb type) even in the case of a flat manifold X.

We are interested here in the question how to add the singular term δ_M concentrated on a zero-dimensional submanifold M of X to the operator $H_U=-\Delta+U$ (this case covers not only quantum fields with point interactions, but also the case when X is a Cartesian product of two

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manifolds, $X=X_0\times Y$, and M has the form $M_0\times Z$ with M_0 being a discrete subset of X_0). If M is a uniformly discrete subset of X and $\dim X\leqslant 3$, then the Green function $G_M(x,y;\zeta)$ of H_M can be obtained through the Krein resolvent formula in terms of the Green function $G_U(x,y;\zeta)$ for H_U.[5,6] An important ingredient of this formula is the so-called "Krein $\mathcal{Q}$-matrix" (a kind of the Dirichlet-to-Neumann map) $Q_{mn}(z)$, $m,n\in M$; under the name "Wigner $\mathcal{R}$-matrix" it appears in the scattering theory[7] and is used in the charge transport theory.[8] To define the diagonal elements of Q for $\dim X>1$ a renormalization procedure is needed. For smooth U, the renormalized Green function $G_U^{\mathrm{ren}}(x,y;\zeta)$, which must be continuous in the whole $X\times X$, is defined as

$$G_U^{\mathrm{ren}}(x,y;\zeta)=G_U(x,y;\zeta)-S(x,y), \tag{1.2}$$

where the "standard singularity" S has the form $S(x,y)=-(1/2\pi)\log d(x,y)$ if $\dim X=2$, and $S(x,y)=1/4\pi d(x,y)$ if $\dim X=3$ [here $d(x,y)$ is the geodesic distance on X]. Now one can set $Q_{mm}(\zeta)=G_U^{\mathrm{ren}}(m,m;\zeta)$. The corresponding renormalization procedure in the Euclidean case is known long ago, see, e.g., Refs. 9 and 10 for the history and the quantum mechanical treatment. It is important to note that usually one obtains $G_U^{\mathrm{ren}}(x,y;\zeta)$ by a momentum cutoff (an ultraviolet regularization procedure); the result is equivalent to that obtained with the help of a dimensional regularization. In the case of brane coupling to gravity or to a gauge field it is necessary to use a dimensional regularization.[11] It is worthy to add that the strict mathematical treatment of the operators (1.1) has its origins in the paper[12] by Berezin and Faddeev. In the case $\dim X\geqslant 4$ there is no regularization procedure involving a singularity independent of the energy parameter ζ (see Example 7 below). Moreover, if U has a Coulomb-type singularity or if an interaction with a gauge field is present, then the function S in (1.2) is different from the standard one, i.e., $S(x,y)\neq 1/4\pi d(x,y)$ (see Examples 12 and 14 below); similar phenomena related to propagation of waves in strongly inhomogeneous media have been studied recently in Ref. 13.

The main goal of our paper is to investigate in detail the singularity of the Green function for the operator $H_U=H_0+U$ where H_0 is the Bochner-Laplace operator on a Riemannian manifold of dimension $\leqslant 3$ and U is a scalar potential from a wide class of measurable functions. As an important consequence we conclude that the operator of the form (1.1) is well defined in this case. It should be stressed that the operators of this form are used not only in the quantum field theory but they occur often in the single-electron theory of condensed matter physics where H_0 represents the Hamiltonian of an electron in the presence of a time-independent magnetic field, U is a confinement electric potential, and δ_M is an additional potential (e.g., the potential of impurities or of a crystal lattice). The Riemannian manifold with nontrivial curvature can appear in this situation, e.g., as a result of the reduction of a few-electron problem to the single-electron one.[14] Another example of using nontrivial three-dimensional Riemannian manifolds is the simulation of the confinement potential of a quantum dot.[15] The defects in solids were investigated previously by methods of quantum gravity in Ref. 16. New technologies of manufacturing two-dimensional nanostructures with nontrivial geometry[17,18] caused the appearance of mathematical models of such structures where, in particular, the Hamiltonian has the form (1.1) with the δ-term simulating the potential of a short range impurity[19] [if the nanostructure is placed in a magnetic field we must replace Δ in (1.1) by the Bochner Laplacian as above]. Moreover, the properties of the Green function G_U are needed for investigation of explicitly solvable models of the geometric scattering theory[20] or spectral theory of periodic hybrid manifolds.[21]

Our analysis of the singularity for the Green function G_U shows that in dimension two the singular term has the standard form even in the presence of an additional $\mathbf{U}(1)$-gauge potential (Theorem 15). On the other hand, in dimension three, S depends on U modulo a Lebesgue class of functions on X (see Theorem 16) and is defined up only to a continuous additive term (the situation here is completely similar to that for the Krein $\mathcal{Q}$-functions, they are defined up to an additive constant). The concrete value of this term is subject of analysis of a given physical problem and is out of the scope of the present work. We mention only that a possible way to fix the corresponding additive constant is to compare the integrated density of states with the trace of G_U^{ren}. At last but not at least we stress that our main results are new *even for the case of Euclidean spaces* $X=\mathbb{R}^n$.

II. DEFINITIONS AND PRELIMINARIES

Throughout the paper we denote by X a complete connected Riemannian manifold of bounded geometry, which means that the injectivity radius r_{inj} of X is positive and every covariant derivative of the Riemann curvature tensor is bounded. Examples are provided by homogeneous spaces with invariant metrics (in particular, Euclidean spaces), compact Riemannian manifolds and their covering manifolds; for discussion of various properties of such manifolds in the context of differential operators we refer to Ref. 22. The dimension of X we denote by ν; the geodesic distance between $x,y\in X$ will be denoted by $d(x,y)$. For $x\in X$ and $r\geqslant 0$ we use the notation $B(x,r)=\{y\in X: d(x,y)<r\}$; throughout the paper, we suppose $r<r_{\text{inj}}$ for radiuses r of all considered sufficiently small balls. For a measurable function f on X, we denote by $\|f\|_p$ the L^p-norm of f. If K is a bounded operator from $L^p(X)$ to $L^q(X)$, $1\leqslant p,q\leqslant\infty$, then its norm will be denoted by $\|K\|_{p,q}$.

Let $A=A_j\,\mathrm{d}x^j$ be a 1-form on X, for simplicity we suppose here $A_j\in C^\infty(X)$. The functions A_j can be considered as the components of the vector potential of a magnetic field on X. On the other hand, A defines a connection ∇_A in the trivial line bundle $X\times\mathbb{C}\to X$, $\nabla_A u=\mathrm{d}u+iuA$; by $-\Delta_A=\nabla_A^*\nabla_A$ we denote the corresponding Bochner Laplacian. In addition, we consider a real-valued scalar potential U of an electric field on X. This potential will be assumed to satisfy the following conditions:

$$U_+ := \max(U,0) \in L^{p0}_{\text{loc}}(X), \quad U_- := \max(-U,0) \in \sum_{i=1}^{n} L^{p_i}(X),$$

$$2\leqslant p_i\leqslant\infty \quad \text{if } \nu\leqslant 3, \quad \nu/2<p_i\leqslant\infty \quad \text{if } \nu\geqslant 4, \quad 0\leqslant i\leqslant n;$$

we stress that p_i as well as n are not fixed and depend on U. The class of such potentials will be denoted by $\mathcal{P}(X)$. Below we will need an approximation of singular potentials by smooth ones; for this purpose the following lemma is useful.

Lemma 1: Let $f\in L^p_{\text{loc}}(X)$, where $1\leqslant p<\infty$, and $f\geqslant 0$. Then there is $g\in C^\infty(X)$ such that $g\geqslant 0$ and $f-g\in L^q(X)$ for all $1\leqslant q\leqslant p$.

Proof: Fix $a\in X$ and for integers n, $n\geqslant 1$, denote $Y_n=B(a,n)\setminus \bar{B}(a,n-1)$. Fix a real sequence a_n, $a_n>0$ such that $\Sigma a_n\leqslant 1$ and denote by f_n the restriction of f to the set Y_n. Since the measure of Y_n is finite, for every n we can find a function g_n, $g_n\in C_0^\infty(X)$, such that $g_n\geqslant 0$, $\operatorname{supp}(g_n)\subset Y_n$, and $\max(\|f_n-g_n\|_p^p,\|f_n-g_n\|_1)\leqslant a_n$. Since the family (Y_n) is locally finite, the pointwise sum $g=\Sigma g_n$ exists and $g\in C_0^\infty(X)$. It is clear that $g\geqslant 0$ and $\max(\|f-g\|_p,\|f-g\|_1)\leqslant 1$, i.e., $f-g\in L^p(X)\cap L^1(X)$. □

We denote by $H_{A,U}$ the operator acting on functions $\phi\in C_0^\infty(X)$ by the rule $H_{A,U}\phi=-\Delta_A\phi+U\phi$. This operator is essentially self-adjoint in $L^2(X)$ and semibounded below,[23] its closure will be also denoted by $H_{A,U}$. By $\operatorname{spec}(H_{A,U})$ we denote the spectrum of $H_{A,U}$ and by $\operatorname{res}(H_{A,U})$ the set of regular points: $\operatorname{res}(H_{A,U})=\mathbb{C}\setminus\operatorname{spec}(H_{A,U})$. Let us denote the resolvent of $H_{A,U}$ by $R_{A,U}(\zeta)$, i.e., $R_{A,U}(\zeta)=(H_{A,U}-\zeta)^{-1}$.

Here we introduce two classes of integral kernels used in the paper. First class, $\mathcal{K}_{\text{cont}}(p)$, $1\leqslant p\leqslant\infty$, consists of all continuous on $X\times X$ functions $K(x,y)$ satisfying for any $r>0$ the condition

$$\lfloor K\rfloor_{p,r} := \max(\operatorname{sup\,ess}_{x\in X}\|\chi_{X\setminus B(x,r)}K(x,\cdot)\|_p, \operatorname{sup\,ess}_{y\in X}\|\chi_{X\setminus B(y,r)}K(\cdot,y)\|_p)<\infty, \tag{2.1}$$

where χ_A stands for the characteristic function of the set $A\subset X$. The second class, $\mathcal{K}(\alpha,p)$, $0\leqslant\alpha<\nu$, $1\leqslant p\leqslant\infty$, consists of all measurable functions K on $X\times X$ obeying the condition (2.1) and

$$|K(x,y)|\leqslant c\max(1,d(x,y)^{-\alpha}) \quad \text{for a constant } c=c(K)>0. \tag{2.2}$$

We set $\mathcal{K}_{\text{cont}}(\alpha,p):=\mathcal{K}(\alpha,p)\cap C(X\times X\setminus D)$, where D is the diagonal $\{(x,y)\in X\times X: x=y\}$.

The above introduced classes of integral kernels are important due to their relations to the properties of the resolvents $R_{A,U}(\zeta)$; these relationships are stated in the following theorem which is our starting point (see Ref. 23, for the proof).

Theorem 2: *For any $\zeta \in \operatorname{res}(H_{A,U})$ the resolvent $R_{A,U}(\zeta)$ has an integral kernel $G_{A,U}(x,y;\zeta)$, the Green function, which belongs to $\mathcal{K}_{\mathrm{cont}}(\lambda,q)$, where q, $1 \leqslant q \leqslant \infty$, is arbitrary, and $\lambda = \nu - 2$ for $\nu > 2$, $\lambda \in (0,\nu)$ is arbitrary for $\nu = 2$, $\lambda = 0$ for $\nu = 1$; moreover, $G_{A,U}$ is continuous in $X \times X$ for $\nu = 1$.*

We should point out that the Green function of a Schrödinger operator can violate the conditions (2.1) and (2.2), if the potential U is not from the class $\mathcal{P}(X)$. Even the decay of the Green function for large distances between x and y (the off-diagonal behavior) can be different from the "standard" exponential one coming from the comparison with the Laplacian; a good example is delivered by the one-dimensional inverse harmonic oscillator, whose Green function has only a polynomial decay at infinity (see Appendix A).

Our further calculations will involve a couple of operations with integral kernels introduced above; here we collect some useful estimates which will be used very intensively.

The well-known Gelfand-Dunford-Pettis theorem claims that if K is a bounded operator from $L^p(X)$ to $L^\infty(X)$ with some p, $1 \leqslant p < \infty$, then it is an integral operator and its kernel $K(x,y)$ satisfies the estimate

$$\sup \operatorname{ess}_{x\in X} \|K(x,\cdot)\|_q < \infty, \quad q = (1 - p^{-1})^{-1}. \tag{2.3}$$

Conversely, if a kernel $K(x,y)$ satisfies (2.3), then it is an integral kernel of a bounded operator from $L^p(X)$ to $L^\infty(X)$.

Lemma 3: Let $K_j : L^{q_j}(X) \to L^\infty(X)$, $1 \leqslant q_j < \infty$, be bounded linear operators with integral kernels $K_j(x,y)$, $j = 1,2$, and $W \in L^{q_1}(X)$, then for a.e. $(x,y) \in X \times X$ the integral $J(x,y) = \int_X K_1(x,z)W(z)K_2(z,y)\mathrm{d}z$ exists and $J(x,y)$ is an integral kernel of the operator K_1WK_2.

Proof: The operator K_1WK_2 is bounded from $L^{q_2}(X)$ to $L^\infty(X)$, therefore, it is an integral operator. Let $f \in L^{q_2}(X) \cap C(X)$ such that $f(x) > 0$ for all $x \in X$. Then there holds

$$K_1WK_2f(x) = \int_X K_1(x,z)W(z)\int_X K_2(z,y)f(y)\mathrm{d}y\,\mathrm{d}z. \tag{2.4}$$

From the other side, according to the estimates (2.3) for K_1 and K_2, there holds

$$\int_X |K_2(\cdot,y)f(y)|\mathrm{d}y \in L^\infty(X), \quad |W(\cdot)|\int_X |K_2(\cdot,y)f(y)|\mathrm{d}y \in L^{q_1}(X),$$

hence,

$$\int_X |K_1(x,z)|\left(|W(z)|\int_X |K_2(z,y)f(y)|\mathrm{d}y\right)\mathrm{d}z < \infty.$$

By the Fubini

$$\int_X \left(\int_X |K_1(x,z)W(z)K_2(z,y)|\mathrm{d}z\right)f(y)\mathrm{d}y < \infty,$$

and since $f(x) > 0$, the inner integral exists for a.e. $(x,y) \in X \times X$.

Let now f be an arbitrary function from $L^{q_2}(X)$. Repeating the arguments above, we get

$$K_1WK_2f(x) = \int_X \left(\int_X K_1(x,z)W(z)K_2(z,y)\mathrm{d}z\right)f(y)\mathrm{d}y \tag{2.5}$$

for a.e. $x \in X$. Therefore J is an integral kernel for K_1WK_2. □

We will often use the estimate given by the lemma below (cf. Ref. 23).

Lemma 4: There exists $r_0>0$ such that for any α, r with $0<r<r_0$, $0\leqslant\alpha<\nu$, and $a,x\in X$ there holds

$$\int_{B(a,r)}\frac{\mathrm{d}y}{d(x,y)^{\alpha}}\leqslant cr^{\nu-\alpha} \tag{2.6}$$

with some $c>0$ depending only on α.

Our next auxiliary result is the following lemma.

Lemma 5: Let $K\in\mathcal{K}(\alpha,p)$, $1\leqslant p<\infty$, $p\alpha<\nu$, and $1/p+1/q=1$, then K is an integral kernel of a bounded operator from $L^q(X)$ to $L^\infty(X)$.

Proof: According to the Gelfand-Dunford-Pettis theorem we must prove

$$\sup\,\mathrm{ess}_{x\in X}\int_X|K(x,y)|^p\,\mathrm{d}y<\infty.$$

Fix r, $0<r<r_0$, and for $x\in X$ expand the integral into two parts,

$$\int_X|K(x,y)|^p\,\mathrm{d}y=\int_{B(x,r)}|K(x,y)|^p\,\mathrm{d}y+\int_{X\setminus B(x,r)}|K(x,y)|^p\,\mathrm{d}y.$$

The first term is estimated by Lemma 4, and the second one is majorated by $\lfloor K\rfloor_{p,r}^p$. □

Lemma 6: Let three measurable functions $K_1(x,y)$, $K_2(x,y)$ and $W(x)$ be given, where $x,y\in X$. Denote $F(x,y,z):=K_1(x,z)W(z)K_2(z,y)$, and if the integral $\int_X F(x,y,z)\mathrm{d}z$ exists, denote it by $J(x,y)$.

(A) *Let $K_j\in\mathcal{K}_{\mathrm{cont}}(\alpha_j,p_j)$, $j=1,2$, and $W\in L^p(X)$, such that $1/p_1+1/p_2+1/p=1$ and $p>\nu/(\nu-\max(\alpha_1,\alpha_2))$. Then $F(x,y,\cdot)\in L^1(X)$ for $x\neq y$, hence J is well defined. Moreover, $J\in\mathcal{K}_{\mathrm{cont}}(\alpha,\infty)$, where $\alpha=\max(p'(\alpha_1+\alpha_2)-\nu,0)$ with $1/p+1/p'=1$, if $p'(\alpha_1+\alpha_2)\neq\nu$, and α is an arbitrary number from $(0,\nu)$ otherwise.*

(B) *Let the conditions of the item* (A) *be satisfied. Assume additionally that $\alpha_1+\alpha_2<\nu$ and $W\in L^q_{\mathrm{loc}}(X)$ with $q>\nu/(\nu-\alpha_1-\alpha_2)$. Then $F(x,y,\cdot)\in L^1(X)$ for any $x,y\in X$ and $J\in C(X\times X)$.*

(C) *Let $W\in L^p(X)$, and $K_1\in\mathcal{K}_{\mathrm{cont}}(p_1)$, $K_2\in\mathcal{K}_{\mathrm{cont}}(\alpha,p_2)$ or $K_1\in\mathcal{K}_{\mathrm{cont}}(\alpha,p_1)$, $K_2\in\mathcal{K}_{\mathrm{cont}}(p_2)$. Assume additionally that $1/p+1/p_1+1/p_2=1$ and $p>\nu/(\nu-\alpha)$. Then $F(x,y,\cdot)\in L^1(X)$ for any $x,y\in X$, and $J\in C(X\times X)$.*

Proof: The proof of the items (A) and (B) is given in Ref. 23.

(C) We give a proof for the case $K_1\in\mathcal{K}_{\mathrm{cont}}(p_1)$ and $K_2\in\mathcal{K}_{\mathrm{cont}}(\alpha,p_2)$; the second case can be considered exactly in the same way.

Let $x,y\in X$; we show first that $F(x,y,\cdot)\in L^1(X)$. Let $r>0$, then for $z\in B(y,r)$ we have

$$|F(x,y,z)|\leqslant ck_1(x,y)W(z)d(y,z)^{-\alpha},\quad k_1(x,y):=\sup_{z\in B(y,r)}K_1(x,z)<\infty,\quad c>0, \tag{2.7}$$

therefore, $F(x,y,\cdot)\in L^1(B(y,r))$ due to the Hölder inequality and our conditions on p. For $z\notin B(y,r)$ due to the Hölder inequality we have the estimate

$$\int_{X\setminus B(y,r)}|F(x,y,z)|\mathrm{d}z\leqslant\left(\int_{X\setminus B(y,r)}|K_1(x,z)|^{p_1}\,\mathrm{d}z\right)^{1/p_1}\lfloor K_2\rfloor_{p_2,r}\|W\|_p,$$

and

$$\int_{X\setminus B(y,r)}|K_1(x,z)|^{p_1}\,\mathrm{d}z\leqslant\int_X|K_1(x,z)|^{p_1}\,\mathrm{d}z=\int_{B(x,r)}|K_1(x,z)|^{p_1}\,\mathrm{d}z+\int_{X\setminus B(x,r)}|K_1(x,z)|^{p_1}\,\mathrm{d}z,$$

where the first term on the right-hand where the first term on the right-hand side is finite due to the continuity of K_1, and the second one is estimated by (2.1). This proves the inclusion $F(x,y,\cdot)\in L^1(X)$.

Now let $x_0, y_0 \in X$, $0<r<R$, and $x\in B(x_0,r/2)$, $y\in B(y_0,r/2)$, then

$$|J(x,y)-J(x_0,y_0)| \leqslant \int_{B(y_0,r)} |F(x,y,z)|\mathrm{d}z + \int_{B(y_0,r)} |F(x_0,y_0,z)|\mathrm{d}x + \int_{X\backslash B(y_0,R)} |F(x,y,z)|\mathrm{d}z + \int_{X\backslash B(y_0,R)} |F(x_0,y_0,z)|\mathrm{d}z + \int_{B(y_0,R)\backslash B(y_0,r)} |F(x,y,z)-F(x_0,y_0,z)|\mathrm{d}z. \tag{2.8}$$

Take $\epsilon>0$ and assume $r<r_0$. For $z\in B(y_0,r)$ we estimate $F(x,y,z)$ as in (2.7), then we get using Lemma 4

$$\int_{B(y_0,r)} |F(x,y,z)|\mathrm{d}z \leqslant c \sup_{\substack{x\in B(x_0,r),\\ y\in B(y_0,r)}} K_1(x,y)\|W\|_p \left[\int_{B(y_0,r)} d(y,z)^{p\alpha/(1-p)}\,\mathrm{d}z\right]^{(p-1)/p} \leqslant C r^{\nu-\alpha-(1/p)} = o(1)$$

as $r\to 0$. On the other hand,

$$\int_{X\backslash B(x_0,R)} |F(x,y,z)|\mathrm{d}z \leqslant \lfloor K_1\rfloor_{p_1,r}\lfloor K_2\rfloor_{p_2,r}\|\chi_{X\backslash B(x_0,R)}W\|_p = o(1) \quad \text{as } R\to\infty.$$

Finally, we conclude that r can be taken sufficiently small and R sufficiently large, such that the sum of the first four terms on the right-hand side of (2.8) is less than $\epsilon/2$. Now it is sufficient to prove that at these fixed r and R the function

$$\int_{B(y_0,R)\backslash B(y_0,r)} F(x,y,z)\mathrm{d}z$$

is continuous as $x\in B(x_0,r/2)$ and $y\in B(y_0,r/2)$. To do this, we note that with some $C'>0$ the following estimate $|F(x,y,z)|\leqslant C'|W(z)|$ takes place for all $x\in B(x_0,r/2)$, $y\in B(y_0,r/2)$, and $z\in B(y_0,R)\backslash B(y_0,r)$. Since $W\in L^1(B(y_0,R)\backslash B(y_0,r))$, the requested continuity follows from the Lebesgue majorization theorem. □

As it was mentioned in the Introduction, we are going to present the Green function in the form

$$G_{A,U}(x,y;\zeta) = S_{A,U}(x,y) + G^{\text{ren}}_{A,U}(x,y;\zeta),$$

where the second term must be continuous in $X\times X$. Such a representation is trivial in the one-dimensional case, the Green function is continuous, and one can set $S_{A,U}\equiv 0$. In dimensions $\nu\geqslant 4$ the problem makes no sense, as the following example shows.

Example 7 (four-dimensional Laplace operator): Consider the simplest case of the Laplacian in $L^2(\mathbb{R}^4)$. The Green function takes the form

$$G(x,y;\zeta) = \frac{\sqrt{-\zeta}}{4\pi^2|x-y|}K_1(\sqrt{-\zeta}|x-y|),$$

where K_1 is the modified Bessel function of the first order. Near the diagonal $x=y$ one has

$$G(x,y;\zeta) = \frac{1}{4\pi^2|x-y|^2} - \frac{\zeta\log|x-y|}{8\pi^2} + k(x,y;\zeta)$$

with a continuous k. Therefore, for $\zeta_1,\zeta_2\in\operatorname{res}(-\Delta)$, $\zeta_1\neq\zeta_2$, the difference

$$G(x,y;\zeta_1) - G(x,y;\zeta_2) \sim \frac{\zeta_2 - \zeta_1}{8\pi^2} \log|x-y|$$

is a discontinuous function, so that the singularity cannot be chosen independent of the spectral parameter.

Therefore, the only nontrivial cases remain $\nu=2$ and $\nu=3$, which we will consider in the present paper.

Example 8 (on-diagonal singularity for the Laplace operator): Here we consider the case $A=0$ and $U=0$, i.e., the case of the Laplace-Beltrami operator $-\Delta$ on the manifold X with $\nu=2$ or $\nu=3$. Denote the Green function of $-\Delta$ by $G(x,y;\zeta)$. Take $y\in X$ and introduce polar coordinates (r_y,ω), $r_y=d(x,y)$, $\omega\in\mathbb{S}^{\nu-1}$, centered at y, then we have in a normal neighborhood W_y of y,

$$-\Delta\psi = -\frac{\partial^2\psi}{\partial r_y^2} + \left(\frac{\nu-1}{r_y} + \theta_y^{-1}\frac{\partial\theta_y}{\partial r_y}\right)\frac{\partial\psi}{\partial r_y},$$

where the function $\theta_y=\theta_y(r_y,\omega)$ is defined in such a way that in W_y, we have $\mathrm{d}x = r_y^{\nu-1}\theta_y(r_y,\omega)\mathrm{d}r_y\,\mathrm{d}\omega$. Since $r_y^{\nu-1}\theta(r_y,\omega)$ is the Jacobian for the inverse to the exponential map in W_y, there holds $\theta_y(0,\omega)\geqslant c_y>0$ and $(\partial/\partial r)\theta_y(0,\omega)=0$ for all $\omega\in\mathbb{S}^{\nu-1}$. Moreover, $\inf c_y>0$ as y runs over a compact set in X.

Denote now

$$S(x,y) = \begin{cases} \dfrac{1}{2\pi}\log\dfrac{1}{d(x,y)}, & \nu=2, \\[2ex] \dfrac{1}{4\pi d(x,y)}, & \nu=3, \end{cases}$$

and for a fixed $\zeta\in\mathrm{res}(-\Delta)$ denote $K(x,y) := G(x,y;\zeta) - S(x,y)$. Then there holds

$$(-\Delta-\zeta)K(\cdot,y) = \theta_y^{-1}\frac{\partial\theta_y}{\partial r_y}\frac{\partial}{\partial r_y}S(\cdot,y) - \zeta S(\cdot,y) =: L(x,y). \tag{2.9}$$

It is clear that $L(\cdot,y)\in L^2(W_y)$, hence due to the Sobolev embedding theorem, $x\mapsto K(x,y)$ is continuous in W_y. Let us show that really $K(x,y)$ is continuous in (x,y). To do this, we fix $y_0\in X$ and take $r_0>0$ such that $B(y_0,2r_0)\subset W_{y_0}$. We prove the following assertion:

(CM) *the map $B(y_0,r_0)\ni y\mapsto L(\cdot,y)\in L^2(B(y_0,r_0))$ is continuous with respect to the norm topology of the space $L^2(B(y_0,r_0))$.*

Let $\chi\in C^\infty(X)$ such that $\operatorname{supp}\chi\subset B(y_0,2r_0)$, $\chi(x)=1$ for $x\in B(y_0,r_0)$, and $0\leqslant\chi(x)\leqslant 1$ for all $x\in X$. Note that $B(y_0,2r_0)$ is a normal neighborhood of y for all $y\in B(y_0,2r_0)$, therefore we can assume that $L(x,y)$ is defined for all $x\in X$ and $y\in B(y_0,2r_0)$. Extend L by zero for $y\notin B(y_0,2r_0)$ and set $T(x,y)=\chi(x)\chi(y)L(x,y)$. It is clear that $T\in\mathcal{K}_{\mathrm{cont}}(\alpha,p)$ where p is arbitrary number with $1\leqslant p\leqslant\infty$, and $\alpha=1$ for $\nu=3$, α is any strictly positive number for $\nu=2$. Using items (A) and (B) of Lemma 6 we can easily show that for every $f\in L^2(X)$ the mapping $B(y_0,r_0)\ni y\to\int_{B(y_0,r_0)}L(x,y)f(y)\mathrm{d}y$ is continuous and the mapping $B(y_0,r_0)\ni y\to\int_{B(y_0,r_0)}|L(x,y)|^2\,\mathrm{d}y$ is also continuous. This proves the assertion (CM). Returning to Eq. (2.9) we see that $K(\cdot,y)$ tends to $K(\cdot,y_0)$ with respect to the topology of $W_2^2(B(y_0,r_0))$. Due to the Sobolev embedding theorem, this implies a uniform convergence in the ball $B(y_0,r)$, i.e.,

$$\lim_{y\to y_0}\sup_{x\in B(y_0,r_0)}|K(x,y)-K(x,y_0)| = 0.$$

This together with the continuity in x proves the required joint continuity in (x,y). Therefore, the functions $S(x,y)$ are suitable on-diagonal singularities of the Laplace operator.

Note that the proof of the separate continuity of the function $K(x,y)$ is considerably simpler and can be found, e.g., in Ref. 24.

III. ON-DIAGONAL BEHAVIOR FOR SINGULAR SCALAR POTENTIALS

Below we will use the notation $L^{p+}_{\mathrm{loc}}(X)=\cup_{q>p}L^q_{\mathrm{loc}}(X)$.

Lemma 9 (singularity is independent of the spectral parameter): Let $\nu=2$ *or* 3, $A\in[C^\infty(X)]^\nu$, $U\in\mathcal{P}(X)$, $\zeta_1,\zeta_2\in\mathrm{res}(H_{A,U})$, *then the difference* $G_{A,U}(x,y;\zeta_1)-G_{A,U}(x,y;\zeta_2)$ *is continuous in* $X\times X$.

Proof: The proof follows from the Hilbert resolvent identity for the kernels, $R_{A,U}(\zeta_1)-R_{A,U}(\zeta_2)=(\zeta_1-\zeta_2)R_{A,U}(\zeta_1)R_{A,U}(\zeta_2)$. The integral kernel $\int_X G_{A,U}(x,z;\zeta_1)G_{A,U}(z,y;\zeta_2)\mathrm{d}z$ of $R_{A,U}(\zeta_1)R_{A,U}(\zeta_2)$ is continuous due to Lemma 6(B). □

The preceding lemma shows that for fixed A and U, the on-diagonal singularity in question exists; for example, as a singularity one can take $G_{A,U}(x,y;\zeta_0)$ for a fixed $\zeta_0\in\mathrm{res}(H_{A,U})$. Our aim is to understand how the singularity depends on A and U.

The following lemma shows that Green functions of Schrödinger operators with smooth potentials have the same on-diagonal singularity.

Lemma 10 (singularity for operator with smooth potentials): Let $\nu=2$ *or* 3, $A\in[C^\infty(X)]^\nu$, $U,V\in\mathcal{P}(X)\cap C^\infty(\Omega)$, *where* Ω *is a domain in* X, *then the difference* $G_{A,U}(x,y;\zeta)-G_{A,V}(x,y;\zeta)$ *has a continuous extension to all points* (x,x), $x\in\Omega$. *In particular, if* $\Omega=X$, *then* $G_{A,U}(x,y;\zeta)-G_{A,V}(x,y;\zeta)\in\mathcal{K}_{\mathrm{cont}}(p)$ *with arbitrary* $p\geqslant 1$.

Proof: Fix a real E sufficiently close to $-\infty$ and take $x_0\in\Omega$. We show that in a neighborhood of (x_0,x_0) in $X\times X$, the difference $F(x,y;E)=G_{A,U}(x,y;E)-G_{A,V}(x,y;E)$ is the restriction of a continuous function in this neighborhood. Due to Lemma 9 the same will hold for all values of the spectral parameter.

Let Ω_0 be a bounded subdomain of Ω and contain x_0; denote $W=U+\chi_{\Omega_0}(V-U)$; it is clear that $W\in\mathcal{P}(X)$. Since $W-U$ is bounded with compact support, one has $R_{A,U}(\zeta)-R_{A,W}(\zeta)=R_{A,U}(\zeta)(W-U)R_{A,W}(\zeta)$, so that the difference

$$G_{A,U}(x,y;E)-G_{A,W}(x,y;E)=\int_X G_{A,U}(x,z;E)(W(z)-U(z))G_{A,W}(z,y;E)\mathrm{d}z$$

is continuous in $X\times X$ according to Lemma 6(B). It remains to show that the function $L(x,y)=G_{A,V}(x,y;E)-G_{A,W}(x,y;E)$ is continuous on $\Omega_0\times\Omega_0$. To do this, let us note that in the sense of distributions the following equality holds:

$$((H_{A,V})_x-E+\overline{(H_{A,V})_y}-E)L(x,y)=(W(x)-V(x))G_{A,W}(x,y;E)+(W(y)-V(y))G_{A,W}(x,y;E), \tag{3.1}$$

where $(H_{A,V})_x$ [respectively, $(H_{A,V})_y$] means that $H_{A,V}$ acts on the first (respectively, the second) argument in L; the bar means that we change the coefficients in $H_{A,V}$ by the complex conjugate ones. The operator in the left-hand side of (3.1) is elliptic in $\Omega_0\times\Omega_0$ with smooth coefficients, while the right-hand term vanishes in $\Omega_0\times\Omega_0$. According to the elliptic regularity theorem L is continuous in $\Omega_0\times\Omega_0$. □

The following Proposition contains our main result on the dependence of the on-diagonal singularity on singularities of the scalar potential.

Proposition 11 (preserving the on-diagonal singularity under singular perturbations): Let $\nu=2$ *or* 3, $A\in[C^\infty(X)]^\nu$, *and* $U_1,U_2\in\mathcal{P}(X)$. *If* $\nu=3$, *assume additionally that* $U_1-U_2\in L^{3+}_{\mathrm{loc}}(X)$. *Then the difference* $G_{A,U_1}(x,y;\zeta)-G_{A,U_2}(x,y;\zeta)$ *is continuous in* $X\times X$ *for any* $\zeta\in\mathrm{res}(H_{A,U_1})\cap\mathrm{res}(H_{A,U_2})$.

Proof: For the sake of brevity we fix A and remove it from the notation, i.e., instead of $G_{A,U}$ we will write G_U, etc.

First of all, using Lemma 1 we choose functions $V_1,V_2\in C^\infty(X)$ semibounded below such that $W_j:=U_j-V_j=\sum_{s=1}^{n_j}W_{j,s}$, where $W_{j,s}\in L^{p_{j,s}}$ with $2\leqslant p_{j,s}<\infty$, $s=1,\ldots,n_j$, $j=1,2$.

For $\zeta \in \mathrm{res}(H_{U_1}) \cap \mathrm{res}(H_{U_2})$ the sets $\mathcal{D}_j := (H_{U_j} - \zeta) C_0^\infty(X)$ are dense in $L^2(X)$, because $C_0^\infty(X)$ is an essential domain of both H_{U_1} and H_{U_2}. As $\psi \in \mathcal{D}_j$, one has

$$R_{U_j}(\zeta)\psi - R_{V_j}(\zeta)\psi = R_{V_j}(\zeta) W_j R_{U_j}(\zeta)\psi. \tag{3.2}$$

As the operators on both sides of (3.2) are bounded and coincide on a dense subset, they coincide everywhere, i.e., (3.2) holds for any $\psi \in L^2(X)$. Combining Lemma 3 and Lemma 6(B) we conclude that in the dimension two, the operator on the right-hand side of (3.2) has a continuous integral kernel, which together with Lemma 10 implies the conclusion of the proposition.

Let us consider the dimension three more carefully. To be shorter, we remove the dependence of the resolvents on ζ from the notation. We have the following chain of equalities:

$$\begin{aligned}R_{U_1} - R_{U_2} &= R_{V_1} - R_{V_2} + R_{V_1} W_1 R_{U_1} - R_{V_2} W_2 R_{U_2} = R_{V_1} - R_{V_2} + R_{V_1} W_1 R_{U_1} + R_{V_2} W_2 (R_{U_1} - R_{U_2}) \\ &\quad - R_{V_2} W_2 R_{U_1} = R_{V_1} - R_{V_2} + R_{V_2} W_2 (R_{U_1} - R_{U_2}) + R_{V_2}(W_1 - W_2) R_{U_1} + (R_{V_1} - R_{V_2}) W_1 R_{U_1}.\end{aligned}$$

Therefore, $(1 - R_{V_2} W_2)(R_{U_1} - R_{U_2}) =: L = A + B + C$, where $A := R_{V_1} - R_{V_2}$, $B := R_{V_2}(W_1 - W_2) R_{U_1}$, $C := (R_{V_1} - R_{V_2}) W_1 R_{U_1}$.

Due to Lemma 10, the operator A has an integral kernel from $\mathcal{K}_{\mathrm{cont}}(p)$ with arbitrary p, $p \geqslant 1$. Since $W_1 - W_2 \in L^{3+}_{\mathrm{loc}}(X)$, the operator B has an integral kernel from $\mathcal{K}_{\mathrm{cont}}(\infty)$ due to Theorem 2 and the items (A), (B) of Lemma 6. As $R_{V_2} - R_{V_1} \in \mathcal{K}_{\mathrm{cont}}(p)$ with arbitrary $p \geqslant 1$ (Lemma 10), the integral kernel for C is from $\mathcal{K}_{\mathrm{cont}}(\infty)$ due to Theorem 2 again and the items (A), (C) of Lemma 6. Therefore, the operator L has an integral kernel $L(x,y) = L(x,y;\zeta) \in \mathcal{K}_{\mathrm{cont}}(\infty)$. Now we note that the multiplication by $W_{2,s}$ is a continuous mapping from $L^\infty(X)$ to $L^{p_{2,s}}(X)$. At the same time, as $G_{V_2} \in \mathcal{K}_{\mathrm{cont}}(1,p)$, $p \geqslant 1$, the resolvent R_{V_2} is a bounded operator from each $L^{p_{2,s}}(X)$ to $L^\infty(X)$ due to Lemma 5. Since $L = (1 - R_{V_2} W_2)(R_{U_1} - R_{U_2})$, we can combine Theorem 2 and Lemma 5 to show that the operator L is a bounded map from $L^p(X)$ to $L^\infty(X)$ for any p with $3/2 < p < \infty$. Since $|L(x,y;\zeta)| = |L(y,x;\bar{\zeta})|$, we see from (2.3) that $L(x,y) \in \mathcal{K}_{\mathrm{cont}}(q)$ for any q with $1 < q < 3$.

One can find ζ such that $\|R_{V_2}(\zeta) W_2\|_{\infty,\infty} =: \alpha < 1$ (see Ref. 23), therefore, the operator $1 - R_{V_2} W_2$ acting in $L^\infty(X)$ is invertible and for any $n \in \mathbb{N}$ there holds

$$R_{U_1} - R_{U_2} = \sum_{k=0}^{n-1} (R_{V_2} W_2)^k L + (1 - R_{V_2} W_2)^{-1} (R_{V_2} W_2)^n L. \tag{3.3}$$

Applying iteratively Lemmas 3 and 6(A) and taking into account Theorem 2, we can show that the operators $(R_{V_2} W_2)^k R_{V_2}$ have integral kernels from $\mathcal{K}_{\mathrm{cont}}(\beta_k, \infty)$ with $\beta_k \leqslant 1$. At the same time, all these operators are bounded from $L^p(X)$ to $L^\infty(X)$ for any p with $3/2 < p < \infty$. Using the same arguments as for L above, we conclude that these kernels are in $\mathcal{K}_{\mathrm{cont}}(\beta_k, q)$ for any q with $1 < q < 3$. Applying now Lemma 6 (C) one proves that the first term on the right-hand side has a continuous integral kernel.

Denote $T_n := (1 - R_{V_2} W_2)^{-1} (R_{V_2} W_2)^{n-1} R_{V_2}$; this operator is bounded from each $L^{p_{j,s}}(X)$ to $L^\infty(X)$; due to the Gelfand-Dunford-Pettis theorem, this is an integral operator with an integral kernel $T_n(x,y)$. The second term in (3.3) takes the form $T_n W_2 L$, and by virtue of Lemma 3 this is also an integral operator with the kernel $S_n(x,y) := \int_X T_n(x,z) W_2(z) L(z,y) \mathrm{d}z$. From the other side, one can write $S_n(x,y) = T_n W_2 l_y(x)$, where $l_y(x) := L(x,y)$. Note that for each $y \in X$ there holds $l_y \in L^\infty(X)$, and the operator $T_n W_2$ is a bounded mapping from $L^\infty(X)$ to $L^\infty(X)$ with the norm $\|T_n W_2\|_{\infty,\infty} \leqslant \|(1 - R_{V_2} W_2)^{-1}\|_{\infty,\infty} \cdot \|R_{V_2} W_2\|^n_{\infty,\infty} \leqslant \alpha^n/(1-\alpha)$.

Now let us fix $x_0 \in X$ and take a bounded open neighborhood Ω of x_0. It is clear that $\|l_y\|_\infty \leqslant c_\Omega$ for all $y \in \Omega$ with a certain $c_\Omega > 0$. Therefore $\sup_{x,y \in \Omega} |S_n(x,y;\zeta)| \leqslant c_\Omega \alpha^n/(1-\alpha)$. Take $\epsilon > 0$ and choose n such that $c_\Omega \alpha^n/(1-\alpha) < \epsilon$. From Eq. (3.3) we have in $\Omega \times \Omega$ the relation $G_{U_1}(x,y;\zeta) - G_{U_2}(x,y;\zeta) = K_n(x,y) + \tau_n(x,y)$, where K_n is continuous and $|S_n| < \epsilon$. As ϵ is arbitrary, this means that $G_{U_1}(x,y;\zeta) - G_{U_2}(x,y;\zeta)$ is continuous in $\Omega \times \Omega$. Since $x_0 \in X$ is arbitrary, the lemma is proven. Due to Lemma 9, this holds for all $\zeta \in \mathrm{res}(H_{V_1}) \cap \mathrm{res}(H_{V_2})$. □

The following example shows that the condition $U_1-U_2\in L^{3+}_{\mathrm{loc}}(X)$ cannot be omitted in dimension three.

Example 12 (Coulomb potential in three dimensions): Let $X=\mathbb{R}^3$, $A=0$, and $U=q/|x|$, i.e., $H\equiv H_{A,U}=-\Delta+q/|x|$. Clearly, $U\notin L^{3+}_{\mathrm{loc}}(\mathbb{R}^3)$. The Green function can be calculated explicitly,[25]

$$G(x,y;\zeta)=\frac{\Gamma(1-\kappa)}{4\pi|x-y|}[W_{\kappa,1/2}(\sqrt{-\zeta}\xi)M'_{\kappa,1/2}(\sqrt{-\zeta}\eta)-W'_{\kappa,1/2}(\sqrt{-\zeta}\xi)M_{\kappa,1/2}(\sqrt{-\zeta}\eta)], \tag{3.4}$$

where $\xi:=|x|+|y|+|x-y|$, $\eta:=|x|+|y|-|x-y|$, $\kappa=-q/\sqrt{-4\zeta}$, $M_{\kappa,1/2}$ and $W_{\kappa,1/2}$ are the Whittaker functions,

$$M_{\kappa,1/2}(x)=e^{x/2}x\Phi(a,2;x),\quad W_{\kappa,1/2}(x)=e^{x/2}x\Psi(a,2;x). \tag{3.5}$$

Here $\Phi(a,c;x)$ and $\Psi(a,c;x)$ are the Kummer function and the Tricomi function, respectively. We prove in Appendix B the asymptotics

$$G(x,0;\zeta)=\frac{1}{4\pi|x|}+\frac{q}{4\pi}\log|x|-\frac{\sqrt{-\zeta}}{4\pi}+\frac{q}{4\pi}\left(\psi\left(1+\frac{q}{2\sqrt{-\zeta}}\right)+\log\sqrt{-\zeta}+\log(2/e)+2C_E\right)+O(|x|\log|x|). \tag{3.6}$$

Therefore, the singularity for $G(x,y;\zeta)$ contains an unavoidable logarithmic term and is different from the standard three-dimensional singularity.

IV. DEPENDENCE OF THE SINGULARITY ON THE MAGNETIC FIELD

Lemma 13 (singularity due to the magnetic field in two dimensions): Let $\nu=2$, then for any $A\in[C^\infty(X)]^\nu$ the difference $G_{A,0}(x,y;\zeta)-G_{0,0}(x,y;\zeta)$ is continuous in $X\times X$ if $\zeta\in\mathrm{res}(H_{A,0})\cap\mathrm{res}(H_{0,0})$.

Proof: Let x_0 be an arbitrary point of X. We show that the difference $G_{A,0}(x,y;\zeta)-G_{0,0}(x,y;\zeta)$ is continuous in a neighborhood of (x_0,x_0) for at least one value of the spectral parameter ζ; due to Lemma 9 this difference is continuous for all admissible spectral parameters.

Take two sufficiently small numbers r and r_0 with $0<r<r_0$. Fix a function $\phi\in C_0^\infty(X)$ such that $\mathrm{supp}\,\phi\subset B(x_0,r_0)$, $\phi(x)=1$ as $x\in B(x_0,r)$. Denote for brevity $H_0:=H_{0,0}$, $H_1:=H_{A,0}$, $H_2:=H_{\phi A,0}$; the corresponding Green functions will be denoted by G_0, G_1, and G_2, respectively.

In $B(x_0,r)\times B(x_0,r)$ for real ζ sufficiently close to $-\infty$ one has in the sense of distributions

$$(((H_1)_x-\zeta)+((\overline{H_2})_y-\zeta))(G_1(x,y;\zeta)-G_2(x,y;\zeta))=0,$$

therefore, due to the elliptic regularity, the difference $G_1(x,y;\zeta)-G_2(x,y;\zeta)$ is continuous in $B(x_0,r)\times B(x_0,r)$. Now we are going to show that $G_2(x,y;\zeta)-G_0(x,y;\zeta)$ is continuous. Since H_0 and H_2 are uniformly elliptic operators with C^∞-bounded coefficients, we are able to use estimates for the Green functions and their derivatives obtained in Ref. 22. First of all,

$$G_0(x,y;\zeta),\quad G_2(x,y;\zeta)\in\mathcal{K}_{\mathrm{cont}}(\lambda,q) \tag{4.1}$$

for arbitrary $\lambda>0$ and $q\in[1,\infty]$ (see Theorem 2). Moreover, for ζ close to $-\infty$ both these kernels are smooth outside the diagonal $x=y$, and according to (Ref. 22, Theorem A1.3.7) we have

$$|\partial_x G_0(x,y;\zeta)|\leqslant C\left(1+\frac{|\log d(x,y)|}{d(x,y)}\right)e^{-\omega d(x,y)},\quad j=1,2,$$

where ∂ is any first order derivative taken in canonical coordinates, and $C,\omega>0$. Additionally, by (Ref. 22, Theorem A1.2.3) for any $p\geqslant1$ there exist $\epsilon,C'>0$ such that

$$\sup_x \int_{d(x,y)>r} |\partial_x G_0(x,y;\zeta)|^p e^{\epsilon d(x,y)}\,\mathrm{d}y + \sup_y \int_{d(x,y)>r} |\partial_x G_0(x,y;\zeta)|^p e^{\epsilon d(x,y)}\,\mathrm{d}x \leqslant C', \quad j=1,2.$$

This implies the inclusion

$$\partial_x G_0(x,y;\zeta) \in \mathcal{K}_{\mathrm{cont}(1+\lambda,q),} \tag{4.2}$$

with the same λ and q as in (4.1).

In canonical coordinates in $B(x_0,r_0)$ both H_0 and H_2 are given by symmetric second-order elliptic expressions with the same principal symbol, in particular, the difference $T:=H_2-H_0$ is defined by a first order differential expression, $T=b_1(x)\partial_1+b_2(x)\partial_2+c(x)$, where b_1, b_1, c are compactly supported smooth functions. For the functions of the form $\psi=(H_0-\zeta)\phi$ with $\phi \in C_0^\infty(X)$ we have $(H_2-\zeta)\phi=(H_0+T-\zeta)R_0(\zeta)\psi=(1+TR_0(\zeta))\psi$, therefore, $R_0(\zeta)\psi-R_2(\zeta)\psi =R_2(\zeta)TR_0(\zeta)\psi$. In terms of integral kernels this means

$$\begin{aligned}\int_X G_0(x,y;\zeta)\psi(y)\mathrm{d}y - \int_X G_2(x,y;\zeta)\psi(y)\mathrm{d}y &= \int_X G_2(x,z;\zeta)[b_1(z)\partial_1 + b_2(z)\partial_2 + c(z)] \\ &\quad \times \int_X G_0(z,y;\zeta)\psi(y)\mathrm{d}y\,\mathrm{d}z \\ &= \int_X G_2(x,z;\zeta)\int_X [b_1(z)K_1(z,y;\zeta) + b_2(z)K_2(z,y;\zeta) \\ &\quad + c(z)G_0(z,y;\zeta)]\psi(y)\mathrm{d}y\,\mathrm{d}z,\end{aligned} \tag{4.3}$$

where

$$K_1(z,y;\zeta) := \partial_{z_1} G_0(z,y;\zeta), \quad K_2(z,y;\zeta) := \partial_{z_2} G_0(z,y;\zeta).$$

According to the general theory of elliptic operators, the set $(H_0-\zeta)C_0^\infty(X)$ is dense in all $L^p(X)$ with any p, $1\leqslant p<\infty$, if ζ is sufficiently close to $-\infty$ (Ref. 22, Sec. A1.2). Due to the estimates (4.1) and (4.2), and Lemma 5, the kernels K_1 and K_2 define bounded operators from $L^q(X)$ to $L^\infty(X)$ for arbitrary $q>2$; denote these operators by $K_1(\zeta)$ and $K_2(\zeta)$. In this notation, the expression on the right-hand side of (4.3) can be rewritten as

$$R_0(\zeta)\psi - R_2(\zeta)\psi = [R_2(\zeta)b_1K_1(\zeta) + R_2(\zeta)b_2K_2(\zeta) + R_2(\zeta)cR(\zeta)]\psi.$$

The operators in both sides are bounded from $L^q(X)$ to $L^\infty(X)$ with any $q>2$ and coincide on a dense subset, therefore, the corresponding kernels coincide, i.e.,

$$\begin{aligned}G_0(x,y;\zeta) - G_2(x,y;\zeta) &= \int_X G_2(x,z;\zeta)b_1(z)K_1(z,y;\zeta)\mathrm{d}z + \int_X G_2(x,z;\zeta)b_2(z)K_2(z,y;\zeta)\mathrm{d}z \\ &\quad + \int_X G_2(x,z;\zeta)c(z)G_0(z,y;\zeta)\mathrm{d}z.\end{aligned} \tag{4.4}$$

By Lemma 6 (B), the function on the right-hand side of (4.4) is continuous. □

The three-dimensional analog of Lemma 13 is not true as the following example shows.

Example 14 (three-dimensional Landau Hamiltonian): Consider in $L^2(\mathbb{R}^3)$ the vector potential of a nonzero uniform magnetic field. By a suitable choice of coordinates one can assume that the field is directed along the x_3 axis, i.e., the magnetic strength vector is $\mathbf{B}=(0,0,2\pi\xi x_3)$, where $\xi >0$ is the density of the magnetic flux through the plane (x_1,x_2). Choose the symmetric gauge for the magnetic vector potential, $\mathbf{A}(\mathbf{x})=\frac{1}{2}\mathbf{B}\times\mathbf{x}$, then $H:=H_{\mathbf{A},0}$ takes the form

$$H=\left(i\frac{\partial}{\partial x_1}-\pi\xi x_2\right)^2+\left(i\frac{\partial}{\partial x_2}+\pi\xi x_1\right)^2-\frac{\partial^2}{\partial x_3^2},$$

and the corresponding Green function is $G(\mathbf{x},\mathbf{y};\zeta)=\Phi(\mathbf{x},\mathbf{y})F(\mathbf{x}-\mathbf{y};\zeta)$, where

$$F(\mathbf{x};\zeta)=\int_0^\infty\frac{\exp[-\pi|\xi|(\mathbf{x}_\perp^2(e^t-1)^{-1}+\mathbf{x}_\parallel^2t^{-1}\ ]}{(1-e^{-t})\exp\left[\left(\frac{1}{2}-\frac{\zeta}{4\pi|\xi|}\right)t\right]\sqrt{t}}\mathrm{d}t, \tag{4.5}$$

$\mathbf{x}_\perp=(x_1,x_2,0)$ and $\mathbf{x}_\parallel=(0,0,x_3)$.[26] In Appendix C we prove the asymptotics

$$G(\mathbf{x},\mathbf{y};\zeta)=\frac{e^{i\pi\xi(\mathbf{x}_\perp\wedge\mathbf{y}_\perp)}}{4\pi|\mathbf{x}-\mathbf{y}|}+\frac{1}{4}\left(\frac{|\xi|}{\pi}\right)^{1/2}Z\left(\frac{1}{2};\frac{1}{2}-\frac{\zeta}{4\pi|\xi|}\right)+o(|\mathbf{x}-\mathbf{y}|) \tag{4.6}$$

as $|\mathbf{x}-\mathbf{y}|\to 0$; here $Z(z;u)$ is the generalized Riemann ζ-function (also known as the Hurwitz ζ-function). Therefore, the on-diagonal asymptotics is

$$S(\mathbf{x},\mathbf{y})=\frac{e^{i\pi\xi(\mathbf{x}_\perp\wedge\mathbf{y}_\perp)}}{4\pi|\mathbf{x}-\mathbf{y}|}=\frac{1}{4\pi|\mathbf{x}-\mathbf{y}|}\exp\left(\frac{i\mathbf{B}(\mathbf{x}\times\mathbf{y})}{2}\right).$$

V. SUMMARY OF RESULTS

We summarize some corollaries from the proven assertions in the following two theorems.

Theorem 15 (on-diagonal singularities of the Green functions in dimension two): *On a two-dimensional manifold of bounded geometry X, for any vector potential $A\in[C^\infty(X)]^2$ and scalar potential $U\in\mathcal{P}(X)$, the Green function $G_{A,U}$ of the Schrödinger operator $H_{A,U}=-\Delta_A+U$ has the same on-diagonal singularity as that for the Laplace-Beltrami operator, i.e.,*

$$G_{A,U}(x,y;\zeta)=\frac{1}{2\pi}\log\frac{1}{d(x,y)}+G_{A,U}^{\mathrm{ren}}(x,y;\zeta),$$

where $G_{A,U}^{\mathrm{ren}}$ is continuous on $X\times X$.

Proof: Proposition 11 shows that the singularity does not depend on the scalar potential $U\in\mathcal{P}(X)$, and Lemma 13 shows that it is independent of the magnetic potential. Therefore, the singularity coincides with that for the Laplacian, see Example 8. □

Theorem 16 (on-diagonal singularities of the Green functions in dimension three): *Let X be a three-dimensional manifold of bounded geometry. For $U\in\mathcal{P}(X)$ and $A\in[C^\infty(X)]^3$ consider the Schrödinger operator $H_{A,U}=-\Delta_A+U$ and its Green function $G_{A,U}(x,y;\zeta)$. If $U_1,U_2\in\mathcal{P}(X)$ and $U_1-U_2\in L^{3+}_{\mathrm{loc}}(X)$, then the Green functions G_{A,U_1} and G_{A,U_2} have the same on-diagonal singularity (i.e., $G_{A,U_1}-G_{A,U_2}$ is continuous in $X\times X$). In particular, for any $U\in\mathcal{P}(X)\cap L^{3+}_{\mathrm{loc}}(X)$ there holds*

$$G_{0,U}(x,y;\zeta)=\frac{1}{4\pi d(x,y)}+G_{0,U}^{\mathrm{ren}}(x,y;\zeta), \tag{5.1}$$

where $G_{0,U}^{\mathrm{ren}}$ is continuous in $X\times X$.

Proof: The theorem is a simple corollary of Proposition 11, and the formula (5.1) follows from Example 8. □

Remark 17: Contrary to the two-dimensional case, the singular term of the Green function for the three-dimensional Schrödinger operator $H_{A,U}$ *does* depend on the scalar potential U as well as on the magnetic vector potential A. In particular, if A is the vector potential of a uniform magnetic field $\mathbf{B}$ in $X=\mathbb{R}^3$, then instead of (5.1) we have

$$G_{A,0}(\mathbf{x},\mathbf{y};\zeta)=\frac{1}{4\pi|\mathbf{x}-\mathbf{y}|}\exp\left(\frac{i\mathbf{B}(\mathbf{x}\times\mathbf{y})}{2}\right)+G_{A,0}^{\mathrm{ren}}(\mathbf{x},\mathbf{y};\zeta),$$

see Example 14. On the other hand, the dependence on scalar potentials is shown in Example 12.

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APPENDIX A: OFF-DIAGONAL ASYMPTOTICS FOR THE INVERSE HARMONIC OSCILLATOR IN DIMENSION ONE

The Green function $G(x,y;\zeta)$ for the inverse harmonic oscillator $H=-d^2/\mathrm{d}x^2-\omega^2x^2/4$, has the form

$$G(x,y;\zeta)=\frac{e^{i\pi/4}\Gamma\left(\frac{1}{2}-i\zeta\right)}{\sqrt{2\pi\omega}}\times U(-i\zeta/\omega,e^{-i\pi/4}\omega^{1/2}\max(x,y))\times U(-i\zeta/\omega,e^{-i\pi/4}\omega^{1/2}\max(-x,-y)), \tag{A1}$$

where $\Im\zeta>0$ and $U(a,x)$ is the Weber function, see (Ref. 27, Chap. 19). Using (Ref. 27, No. 19.8.1), for large z one obtains $U(a,z)=e^{-z^2/4}z^{-1/2-a}u(z)$, where $\lim_{z\to\infty}u(z)=1$. Returning to the Green function we see that for fixed x and large y one has (assuming $y>x$)

$$G(x,y;\zeta)=\frac{e^{i\pi/4}\Gamma\left(\frac{1}{2}-i\zeta\right)}{\sqrt{2\pi\omega}}U(-i\zeta/\omega,-e^{-i\pi/4}\omega^{1/2}x)\frac{e^{i\omega y^2/4}}{(e^{-i\pi/4}\omega^{1/2}y)^{-i\zeta/\omega+(1/2)}}v(y),$$

where $\lim_{y\to\infty}v(y)\neq 0$. Therefore, for large $|x-y|$ the Green function has only a polynomial decay.

APPENDIX B: ON-DIAGONAL SINGULARITY FOR THE COULOMB HAMILTONIAN

Here we prove the asymptotics (3.6).

We are interested in asymptotics of the functions $x\mapsto G(x,x_0;\zeta)$ as $x\to x_0$ at fixed $\zeta\in\mathrm{res}(H)$ and $x_0\in\mathbb{R}^3$. As the potential is smooth outside the origin, the Green function has the standard on-diagonal asymptotics if $x_0\neq 0$. We consider the case $x_0=0$. We have $M_{\kappa,1/2}(0)=0$, $M'_{\kappa,1/2}(0)=1$, therefore,

$$G(x,0;\zeta)=\frac{\Gamma(1-\kappa)}{4\pi|x|}W_{\kappa,1/2}(2\sqrt{-\zeta}|x|).$$

Consider the following expansions [cf. items 6.1(1) and 6.8(13) in Ref. 28]:

$$\Phi(a,2;x)=1+\frac{a}{2}x+\frac{a(a+1)}{12}x^2+\cdots,$$

$$\Psi(a,2;x)=\frac{1}{x\Gamma(a)}+\Phi(a,2;x)\log x+\sum_{k=0}^{\infty}\frac{\Gamma(a+k)[\psi(a+k)-\psi(1+k)-\psi(2+k)]}{\Gamma(a)(k+1)!k!}x^k$$
$$=A_{-1}x^{-1}+A_0+A_1x+A_2x^2+\cdots+B_0\log x+B_1x\log x+B_2x^2\log x+\cdots,$$

where

$$A_{-1}=\frac{1}{\Gamma(a)},\quad A_0=\frac{\psi(a)-\psi(1)-\psi(2)}{\Gamma(a-1)},\quad A_1=\frac{a(\psi(a+1)-\psi(2)-\psi(3))}{2\Gamma(a-1)},$$

$$A_2 = \frac{a(a+1)(\psi(a+2)-\psi(3)-\psi(4))}{12\Gamma(a-1)}, \quad B_0 = \frac{1}{\Gamma(a-1)}, \quad B_0 = \frac{a}{2\Gamma(a-1)}, \quad B_2 = \frac{a(a+1)}{12\Gamma(a-1)}.$$

Using (3.5), we get

$$\begin{aligned} W_{\kappa,1/2}(x) &= A_{-1} + \left(A_0 - \frac{1}{2}A_{-1}\right)x + B_0 x \log x + O(|x^2 \log x|) \\ &= \frac{1}{\Gamma(a)} + \left(\frac{\psi(a)-\psi(1)-\psi(2)}{\Gamma(a-1)} - \frac{1}{2\Gamma(a)}\right)x + \frac{1}{\Gamma(a-1)}x \log x + O(|x^2 \log x|). \end{aligned}$$

Since $\psi(1) = -C_E$, $\psi(2) = 1 - C_E$, where C_E is the Euler constant, we get (3.6) after some trivial algebra.

APPENDIX C: ON-DIAGONAL SINGULARITY OF THE THREE-DIMENSIONAL LANDAU HAMILTONIAN

In this appendix, we are going to prove the asymptotics (4.6).

Set in the integral (4.5) $\mathbf{x}_\perp = 0$ and denote $\mathbf{x}_\parallel = z$. Then after the change of variables $t \to t^2$ in this integral, we obtain

$$G(0,0,z;0,0,0;\zeta) = \frac{|\xi|^{1/2}}{2\pi}\int_0^\infty \frac{\exp(-az^2t^{-2} - ct^2)}{1 - e^{-t^2}}\mathrm{d}t, \tag{C1}$$

where $a = \pi|\xi|$ and $c = (1/2) - (\zeta/4\pi|\xi|)$. Represent now $G(0,0,z;0,0,0;\zeta) = f_1(z;\zeta) + f_2(z;\zeta)$, where

$$f_1(z;\zeta) = \frac{|\xi|^{1/2}}{2\pi}\int_0^\infty \frac{\exp(-az^2t^{-2} - ct^2)}{t^2}\mathrm{d}t,$$

$$f_2(z;\zeta) = \frac{|\xi|^{1/2}}{2\pi}\int_0^\infty \left(\frac{1}{1 - e^{-t^2}} - \frac{1}{t^2}\right)\exp(-az^2t^{-2} - ct^2)\mathrm{d}t. \tag{C2}$$

Changing the variable $t \to t^{-1}$ and using the relation

$$\int_0^\infty \exp(-bt^2 - c/t^2)\mathrm{d}t = \frac{1}{2}(\pi/b)^{1/2}\exp(-2(bc)^{1/2})$$

(see Ref. 29, Sec. V. I, formula 2.3.16.3), we obtain $f_1(z;\zeta) = \exp(-(2\pi|\xi| - \zeta)^{1/2}|z|)/(4\pi|z|)$, or $G(0,0,z;0,0,0;\zeta) = (4\pi|z|)^{-1} + g(z;\zeta)$, where

$$g(z;\zeta) = -\frac{1}{4\pi}(2\pi|\xi| - \zeta)^{1/2} + f_2(z;\zeta). \tag{C3}$$

It is clear that the function g is continuous with respect to z and analytic with respect to ζ, $\zeta \in \mathrm{res}(H_{A,0})$. We can rewrite (C1) in the form

$$\frac{|\xi|^{1/2}}{2\pi}\int_0^\infty \frac{\exp(-\pi|\xi|z^2t^{-1})}{(1 - e^{-t})\exp\left(\left(\frac{1}{2} - \frac{\zeta}{4\pi|\xi|}\right)t\right)\sqrt{t}}\mathrm{d}t = \frac{1}{4\pi|z|} + g(z;\zeta). \tag{C4}$$

Let $h(t) = (e^t - 1)^{-1} - t^{-1}$; the function h is real analytic on the whole line, $h(t) \to 0$ as $t \to +\infty$ and $h(t) \to -1$ as $t \to -\infty$. Therefore, h is bounded on $\mathbb{R}$. Let us represent $F(\mathbf{x};\zeta)$ in the form

$$F(\mathbf{x};\zeta)=\int_0^\infty \frac{\exp(-\pi|\xi|\mathbf{x}^2t^{-1})}{(1-e^{-t})\exp\left[\left(\frac{1}{2}-\frac{\zeta}{4\pi|\xi|}\right)t\right]\sqrt{t}}\mathrm{d}t+\int_0^\infty \frac{\exp(-\pi|\xi|\mathbf{x}^2t^{-1})}{(1-e^{-t})\exp\left[\left(\frac{1}{2}-\frac{\zeta}{4\pi|\xi|}\right)t\right]\sqrt{t}}$$
$$\times\{\exp[-\pi|\xi|\mathbf{x}_\perp h(t)]-1\}\mathrm{d}t\equiv I_1(\mathbf{x},\zeta)+I_2(\mathbf{x},\zeta). \tag{C5}$$

It is easy to show that I_2 is a continuous function in the domain $\mathbf{x}\in\mathbb{R}^3$, Re $\zeta<2\pi|\xi|$. Let us show that $I_2(\mathbf{x},\zeta)\to 0$ locally uniformly with respect to ζ, Re $\zeta<2\pi|\xi|$, as $\mathbf{x}\to 0$. It is sufficient to show that

$$A(\mathbf{x},\zeta)\equiv\int_0^\infty \frac{\exp(-\pi|\xi|\mathbf{x}^2t^{-1})}{(1-e^{-t})\exp\left[\left(\frac{1}{2}-\frac{\zeta}{4\pi|\xi|}\right)t\right]\sqrt{t}}|\exp[-\pi|\xi|\mathbf{x}_\perp^2h(t)]-1|\mathrm{d}t\to 0$$

locally uniformly with respect to $\zeta\in\mathbb{R}$, $\zeta<2\pi|\xi|$, as $\mathbf{x}\to 0$. Fix $\zeta\in\mathbb{R}$, $\zeta<2\pi|\xi|$. Since $\mathbf{x}_\perp^2\leqslant\mathbf{x}^2$, we have $|\exp[-\pi|\xi|\mathbf{x}_\perp^2h(t)]-1|\leqslant\mathrm{const}\,\mathbf{x}^2$ in a neighborhood of the point $(0,0,z)$. Therefore, using (C4), we get

$$A(\mathbf{x},\zeta)\leqslant c\mathbf{x}^2\int_0^\infty \frac{\exp(-\pi|\xi|\mathbf{x}^2t^{-1})}{(1-e^{-t})\exp\left[\left(\frac{1}{2}-\frac{\zeta}{4\pi|\xi|}\right)t\right]\sqrt{t}}\mathrm{d}t\leqslant\frac{|\mathbf{x}|}{|\xi|^{1/2}}+\frac{c\mathbf{x}^2}{|\xi|^{1/2}}f(|\mathbf{x}|,\zeta),$$

and we get the required limit. Using (C4) again, we obtain

$$I_1(|\mathbf{x}|,\zeta)=\frac{1}{|\xi|^{1/2}|\mathbf{x}|}+f(|\mathbf{x}|,\zeta). \tag{C6}$$

Using (C5) and (C6) we get

$$G(\mathbf{x},\mathbf{y};\zeta)=\frac{1}{4\pi}\frac{\exp[\pi i\xi(\mathbf{x}_\perp\wedge\mathbf{y}_\perp)]}{|\mathbf{x}-\mathbf{y}|}+\widetilde{F}(\mathbf{x},\mathbf{y};\zeta),$$

where $\widetilde{F}(\mathbf{x},\mathbf{y};\zeta)$ is jointly continuous with respect to $(\mathbf{x},\mathbf{y})\in\mathbb{R}^3\times\mathbb{R}^3$ for all $\zeta\in\mathrm{res}(H_{\mathbf{A},0})$.

Denote $Q(\zeta)=\lim_{|\mathbf{x}-\mathbf{y}|\to 0}\widetilde{F}(\mathbf{x},\mathbf{y};\zeta)$; this limit is independent of $\mathbf{x}$ and $\mathbf{y}$ since $\widetilde{F}(\mathbf{x},\mathbf{y};\zeta)$ is invariant with respect to magnetic translations $T_\mathbf{a}$, $\mathbf{a}\in\mathbb{R}^3: T_\mathbf{a}f(\mathbf{x})=\exp[\pi i\xi(\mathbf{a}_\perp\wedge\mathbf{x}_\perp)]f(\mathbf{x}-\mathbf{a})$. From (4.5) we obtain

$$\frac{\partial}{\partial\zeta}Q(\zeta)=\frac{1}{16\pi^2|\xi|^{1/2}}\int_0^\infty \exp\left[\left(\frac{1}{2}-\frac{\zeta}{4\pi|\xi|}\right)t\right](1-e^{-t})^{-1}\sqrt{t}\,\mathrm{d}t.$$

Using Eq. (1.10.4) from Ref. 28 we get $\int_0^\infty t^{s-1}e^{-vt}(1-e^{-t})^{-1}\,\mathrm{d}t=\Gamma(s)Z(s,v)$ and the obvious relation $\partial Z(s,v)/\partial v=-sZ(s+1,v)$ implies immediately

$$Q(\zeta)=\frac{1}{4}\left(\frac{|\xi|}{\pi}\right)^{1/2}Z\left(\frac{1}{2};\frac{1}{2}-\frac{\zeta}{4\pi|\xi|}\right)+C \tag{C7}$$

with a constant $C\in\mathbb{R}$. To determine C we compare (C7) with (C3) in the limit $\Re\zeta\to-\infty$. Since $Q(\zeta)=g(0;\zeta)$, we have from (C3) and (C2),

$$Q(\zeta)-\frac{1}{4\pi}(2\pi|\xi|-\zeta)^{1/2}\to 0 \quad \text{as } \Re\zeta\to-\infty.$$

On the other hand, by the Hermite relation [see (1.10.7) from Ref. 28] there holds $Z(1/2,v)+2v^{1/2}\to 0$ as $\Re v\to+\infty$. Comparing the two last relations with (C7), we get $C=0$. Thus, (4.6) is proven. Note that the expression for $Q(\zeta)$ was obtained at the physical level of rigor in Ref. 30 and can be found also in Ref. 9.

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