

SINGULAR POTENTIALS AND PERTURBATION THEORY

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The perturbation theory for ordinary differential operators with singular potentials is studied on simple examples. Singular potentials induce a change of asymptotic behaviour of eigenfunctions near the singularity. This effect is to some extent analogous to a change of boundary conditions, and gives rise to "counterterms" in the perturbation theory formulae. We show also that the analyticity of eigenfunctions in the coupling constant is not equivalent, generally, to the analyticity of the corresponding operator in the Hilbert space in any reasonable sense.

СИНГУЛЯРНЫЕ ПОТЕНЦИАЛЫ И ТЕОРИЯ ВОЗМУЩЕНИЙ

В работе на простых примерах изучается теория возмущений для обыкновенных дифференциальных операторов с сингулярными потенциалами. Сингулярные потенциалы вызывают изменение асимптотического поведения собственных функций вблизи особой точки. Это явление до некоторой степени аналогично изменению граничных условий и приводит к появлению «контрчленов» в формулах теории возмущений. Показано также, что аналитичность собственных функций по константе связи в общем не эквивалентна аналитичности соответствующего оператора в гильбертовом пространстве.

I. INTRODUCTION

It is a well-known fact [1] that the formal perturbation theory leads to divergent results in the case of the Schrödinger problem

$$-u''(x) + q(x)u(x) = k^2u(x), \quad (1)$$

with the potential q singular at least as x^{-2} in the point $x = 0$. In the present paper we show on examples how to overcome this complication in the case of absolutely continuous spectra. Isolated eigenvalues of singular differential operators have been studied recently in [2].

We believe there are two reasons which make this problem topical: 1. There is a chance to get a better insight into complications of more realistic physical theories

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dealing with unbounded operators, e.g. second-quantized theories. 2. We can get some idea about the consequences of changed asymptotic and analytic properties [1, 3] of the system in the singular region.

Although a number of physical applications of singular potentials is known, the main purpose of this paper is to show what new effects to expect for physical systems with complicated mathematical properties (see below) of generalized eigenfunctions (GE) belonging to the continuous spectrum in the coupling constant g . In this paper we consider real analyticity only. The complex analyticity (complex g) may be treated in a quite analogous way. The standard questions of the theory of differential operators are presented in a somewhat simplified form; for details see, e.g., [4—9].

Note. Below we employ the symbol $f \sim v(x)$ to express $f = \text{const } v(x) + \text{higher terms in } x, x \rightarrow 0$.

II. PERTURBATION THEORY FOR x^{-2} -LIKE POTENTIALS

One of the most important tasks of the perturbation theory is to find asymptotic or even analytic expansions in powers of a small parameter (coupling constant) g for quantities of physical interest. The problem becomes a difficult one for singular (unbounded) interactions. In physical theories we know the region in the space of variables where the singularity is concentrated. An interesting case occurs when the asymptotic or analytic behaviour of basic physical objects (eigenfunctions [4—7], Green and correlation functions [1, 3]) in this region is changed. In many cases, this change indicates a change of the domain of the Hamiltonian in its Hilbert space [7]. In local theories it is sufficient to know a set of boundary conditions on a surface surrounding the singularity. These boundary conditions are g -dependent and reveal the asymptotic properties we have mentioned. In final results, the surface is to be removed by a limit passage. To obtain a correct perturbation theory, we have to expand the boundary conditions in g as well. The last fact is often obscured by formal regularization methods, e.g. cutoffs. We shall call the terms we get in this way due to the g -dependent asymptotic conditions — counterterms. Nonsingular conditions can lead to singular counterterms as the example $\varepsilon^a = \exp(g \ln \varepsilon)$, $\varepsilon \rightarrow 0, g > 0$ shows.

The above discussion may be illustrated by the example of Eq. (1). The latter is equivalent to the integral equation

$$u(x) = u(\varepsilon) \cos k(x - \varepsilon) + u'(\varepsilon) k^{-1} \sin k(x - \varepsilon) + k^{-1} \int_{\varepsilon}^x u(y) q(y) \sin k(x - y) dy. \quad (2)$$

Eq. (2) forms the starting point for the perturbation theory for potentials with an isolated singularity in the point $x = 0$. Let us consider the potential

$$q(x) = g(g + 1)x^{-2} + V(x). \quad (3)$$

The potential $V(x)$ is supposed to be continuous on $[0, \infty)$. We suppose also $q(x)$ decreases sufficiently quickly for $x \rightarrow \infty$. Then the operator (1), (3) has an absolutely continuous spectrum $E = k^2 \geq 0$, with GE which behave like $\sin(kx + \delta)$ [8]. Consequently, we can study also the scattering matrix $S(k, g) = \exp(2i\delta)$. The choice $g(g + 1)$ of the coupling constant is very convenient for our purpose, although it is not obvious. Properties of the operator (1), (3) have been studied by many authors, see [4—9] and references given therein. The potential (3) has been studied within both one-dimensional models and the quantum mechanical scattering theory. In the latter case Eq. (1) can be considered as the radial Schrödinger equation for a particle with a definite angular momentum. It is interesting to mention that the predictions of classical mechanics and quantum physics are quite different in this case. According to classical mechanics, the particle “falls” into the singularity for $g < 0$ (attractive potential), which has no analogy in quantum mechanics, for $g \geq -1/2$ at least [6, 7].

We shall recall only a few basic facts which hold true for sufficiently small values of $|g|$.

To define a selfadjoint operator in the Hilbert space $L_2((0, \infty), dx)$ we have to add an asymptotic condition in $x = 0$. This condition is fulfilled by any function from the domain of this operator [7], and also by its GE [5]. There are two independent conditions

$$f_1 \sim x^{1+a}, \quad f_2 \sim x^{-a}. \quad (4)$$

Any linear combination

$$f \sim x^{1+a} + \Lambda(g)x^{-a} \quad (5)$$

with real $\Lambda(g)$ defines a selfadjoint g -parametric operator family [7]. We put $f \sim x^{-a}$ for $\Lambda(g) = \infty$. For $\Lambda(g)$ analytic, GE are analytic in g as well. For $g = 0$, (5) passes into the standard condition $\Lambda(0)u'(0) - u(0) = 0$.

Let us put $\Lambda(g) = 0$ in (5). This most natural condition [6, 7] is known from the Regge theory, too [8]. The analyticity of this operator family for $V(x) = 0$ has been discussed by Kato [9] (Chap. VII, Example 4.15).

The simple shift $\lambda = g + 1/2$ leads to common parametrization $\lambda^2 - 1/4$ instead of $g(g + 1)$ [8]. The inclusion of the potential $V(x)$ into the perturbation causes no changes either in the general results of the Regge theory or in their proofs.

We shall construct a perturbation theory for the GE of this operator. As the energy values are g -independent for the continuous spectrum, the theory simplifies. The result is given by the following

Theorem: Let $u(x)$ be the GE of the operator (1), (3), (5) with $\Lambda(g) = 0$, normalized by the condition $u(x) = (1 + g)^{-1} \times (kx)^{1+a} + o(x^{1+a})$, $x \rightarrow 0$. $u(x)$ is

analytic in g for $x > 0$: $u = \sum_{n=0}^{\infty} g^n u_n$. The n -th approximation of u is given by the formulae

$$u_0 = u(g=0) = \sin kx, \quad (6)$$

$$u_1 = \lim_{\varepsilon \rightarrow 0} [F(u_0) + \ln(k\varepsilon) \sin kx], \quad (7)$$

$$u_n = \lim_{\varepsilon \rightarrow 0} [F(u_{n-1}) + F(u_{n-2}) + (n-1)^{-1} \ln^n(k\varepsilon) \sin kx], \quad n \geq 2. \quad (8)$$

(We have denoted $F(v) = k^{-1} \int_{\varepsilon}^x (v^{-2} + V(y))v(y) \sin k(x-y) dy$.)

Proof: The analyticity of u in g is proved by the same method as in Theorem 7.2.1 in [8]. Now let us suppose for a moment that $V(x)$ in (3) is analytic in x near $x=0$. We have $u = (1+g)^{-1}(kx)^{1+\alpha} + r(x)$, $r(x) = O(x^{2+\alpha})$. Let us substitute this result into (2) for the boundary conditions in the point ε . The standard expansion of both sides of (2) in powers of g [9] gives (6)–(8) up to the form of the counterterms. Now let us perform the limit passage $\varepsilon \rightarrow 0$. We need not bother about the existence of the limit, because the correction of the given order in g actually independent on ε . By using the structure of $r(\varepsilon)$ [4] we find that only the expansion of the term $(k\varepsilon)^{\alpha} \sin kx$ is not ruled out. This gives (6)–(8). Results for general $V(x)$ may be proved easily by a limit passage.

For large values of x , $u(x)$ behaves, of course, like $A(g) \sin(kx + \delta)$. The amplitude depends on $V(x)$. In such a way we can find from the results of the theorem the phase shift and the scattering matrix elements of any order in g .

III. QUESTIONS OF ANALYTICITY

In the previous example we have been able to construct selfadjoint families of operators with GE analytic in g . The situation is quite different with the potential

$$q(x) = gx^{-4}. \quad (9)$$

The operator (1), (9) has been studied in [10, 11]. We shall add only a few remarks concerning the results of [11]. In analogy with Eq. (4) the asymptotic conditions near $x=0$ are

$$f_1 \sim x \cosh \frac{\sqrt{g}}{x}, \quad f_2 \sim \frac{x}{\sqrt{g}} \sinh \frac{\sqrt{g}}{x}. \quad (10)$$

They are analytic in g and pass into the conditions $u(0)=0$ and $u'(0)=0$ for $g=0$. For $g \leq 0$, any real combination of conditions (10) defines a selfadjoint operator

family in $L_2((0, \infty), dx)$. However, for $g > 0$, the only admissible behaviour of GE is a nonanalytic one [11]:

$$f \sim x \exp\left(-\frac{\sqrt{g}}{x}\right). \quad (11)$$

This condition defines a nonselfadjoint operator for $g < 0$. For $g > 0$, (11) plays no role in the definition of the domain of the corresponding operator. This happens because the limit point case [4, 5] occurs in $x=0$.

For $g < 0$, the corresponding Hamiltonians are not bounded from below. Indeed, it is possible to prove that they possess (besides the obvious continuous spectrum $E = k^2 \geq 0$) an infinite sequence of bounded states with an arbitrary big negative energy. Only unstable systems could be described by such operators without the ground state. This has been made in [10] where a nonselfadjoint asymptotic condition is employed to study the trapping of a particle.

The perturbation theory is constructed in analogy with the preceding section. Now, however, the simple asymptotes (10), (11) do not provide sufficient information to find all the counterterms. In fact, it would be necessary to study the singularity of GE in detail by using methods of singular differential equations of the second kind [4]. In the case of (11), we have to construct the perturbative expansion in powers of \sqrt{g} : $u = \sum_{n=0}^{\infty} g^{n/2} u_n$.

In other words, the solution is analytic in the variable \sqrt{g} .

Clearly, even and odd terms in this series are not coupled by the perturbation. Consequently, we have to know both terms, u_0 , u_1 , of this expansion. The comparison of (10) and (11) gives $u_0 = \sin kx$, $u_1 = \cos kx$.

Despite the fact that the solution is nonanalytic for $g > 0$, we can formally define another scattering operator by means of the phase shift of the analytic "GE" with the "wrong" asymptotes, cf. (10). This example shows that convergence or even analyticity of the perturbation theory series for some quantity does not prove the existence of the perturbed theory in the Hilbert space. In our example we are able to construct a "scattering operator", which for $g > 0$ is not connected with the Hamiltonian in the Hilbert space. Indeed, to study the analyticity of an operator family, more elaborate definitions of analyticity are necessary [9].

IV. CONCLUSIONS

We have seen that counterterms arise naturally in the singular perturbation theory due to the varying asymptotic conditions. The explicit form of the perturbation theory will, nevertheless, differ strongly for various types of singularity of eigenfunctions. In the case of the branching point (Sect. 2), the situation

appears to be comparatively simple. For eigenfunctions essentially singular at $x = 0$ (cf. Sect. 3.; essential singularity combines with the branching point in the general case) cumbersome computations would be inevitable to find all the counterterms. The situation is analogous to the difference between the singular equations of the first and the second kind [4].

In the latter case, another complication can take place. The analytic solution in g can have no interpretation within the framework of the Hilbert space theory (Sect. 3). Hence, using formal "renormalized" expansion in powers of g , we can abandon the axioms of quantum mechanics. The physically interesting solutions are in this case nonanalytic in g [2, 11]. The last fact complicates enormously the perturbation methods for this type of problems.

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REFERENCES

- [1] Graeber, R., Dürr, P. H.: *Nuovo Cim. A* 40 (1977), 11.
- [2] Harrell, E. M.: *Ann. Physics* 105 (1977), 379.
- [3] Wilson, K. G., Kogut, J.: *Phys. Rep.* 12 C (1974), 75.
- [4] Coddington, E. A., Levinson, N.: *Theory of Ordinary Differential Equations*. McGraw-Hill, New York 1955.
- [5] Levitan, B. M., Sargsyan, I. S.: *Vvedenie v spektralnyu teoriyu*. Nauka, Moscow 1970.
- [6] Narnhofer, A.: *Acta Phys. Austr.* 40 (1974), 306.
- [7] Pick, Š.: *J. Math. Phys.* 18 (1977), 118.
- [8] Nussenzweig, H. M.: *Causality and Dispersion Relations*. Academic Press, New York 1972.
- [9] Kato, T.: *Perturbation Theory for Linear Operators*. Springer Verlag, Berlin 1966.
- [10] Vogt, E., Wannier, G.: *Phys. Rev.* 95 (1954), 1190.
- [11] Calogero, R.: *Variable Phase Approach to Potential Scattering*. Academic Press, New York 1967.

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