Associative algebras of generalized functions and their application in quantum mechanics

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The paper reviews the last investigations made by Yu. M. Shirokov, devoted to associative algebras of generalized functions and their application in quantum mechanics. Associative algebras of functionals, including the δ function and also the elements $\epsilon = \text{sign } x$ (in the one-dimensional case) and $r = |x|$ (in the three-dimensional) are constructed. A method of solving quantum problems with δ potentials is explained and illustrated by some examples. The representation of free solutions of the Schrödinger equation with singular δ potentials is described.

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INTRODUCTION

Shirokov frequently emphasized that one of the main mathematical difficulties of relativistic quantum field thoery is the definition of the correct operation of multiplication of field operators. In recent years, he concluded that this difficulty could be overcome by the construction of associative algebras of generalized functions of a certain class.[1] The simplest models that imitate the quantum-field problems, in particular, the problem of ultraviolet divergences, are the models of quantum mechanics described by singular concentrated (δ-functional) potentials. The solution of problems associated with these potentials then led to the construction of associative algerbras of generalized functions of one and three variables and to their subsequent application.[1-9]

The main difficulty in the formulation of such problems is that the most concentrated potentials do not define linear operators on a Hilbert space. The problem in this case consists of giving an operator meaning to the total Hamiltonian $H = H_0 + V$ with interaction. In physics investigations, singular potentials of such type are, as a rule, specified by means of boundary conditions, and great efforts are needed to construct their operator realization, which is frequently altogether absent.

The first mathematical investigation of this problem, for the example of a particle in the field of a concentrated potential in three dimensions, was made in Ref. 10. The method used there was generalized in Ref. 11 to the case of the three-body problem with two-body δ potentials, which corresponds to the model constructed in Ref. 12. The scheme for the construction of Hamiltonians corresponding to δ potentials proposed in Refs. 10 and 11 consists of finding self-adjoint extensions of the kinetic-energy operator H_0 from a suitable subspace in the space L_2 of square-integrable functions. Additional considerations are invoked to choose physically acceptable extensions. In the case of one dimension, the n-particle problem with two-body δ potentials was solved in Ref. 13. The formulation of the one-dimensional problem is much simpler than the many-dimensional one and does not in fact require the use of the theory of extensions. The approach was developed further, but from a different point of view—by means of extensions through the ground state—in Refs. 14 and 15. In Refs. 15 and 16, the problem of regularizing δ Hamiltonians by regular Hamiltonians was investigated. In Ref. 16 there is a generalization of the model of Ref. 10 to the case of a particle in the field of several singular centers.

A different approach to the construction of dynamical models with δ potentials with an algebraic basis and using the ideas of "nonstandard analysis" was proposed in Ref. 17. However, it has not yet proved possible to construct new examples on the basis of this approach. The construction of a singular dynamics through modification of the evolution operator is the subject of Ref. 18.

The approach proposed by Shirokov in Refs. 3 and 4 using algebras of generalized functions differs from preceding approaches in that one does not define a Hamiltonian operatir on a space of square-integrable functions, but rather a pair $\{\mathcal{H}, H\}$ is constructed in a self-consistent manner: a Hilbert space $\mathcal{H}$ (not necessarily L_2) and a Hamiltonian H that acts on it. Such an approach augments the list of models with δ-functional potentials. In this way it was possible to construct models with a nontrivial spectral structure. For example, models with potentials of the type δ' and $\Delta\delta$ in spaces $\mathcal{H} \neq L_2$ were realized.[3,4] Such problems can also be solved by the methods of the theory of extensions that go beyond the original space. But it is necessary to answer two questions: Extension to where? And how? Also nontrivial in this case is the problem of the regularization of singular potentials by regular potentials.

The method of solving quantum-mechanical problems with δ-functional potentials developed by Shirokov in

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Refs. 3 and 4 is based on the use of associative algebra of generalized functions that contain functionals such as the δ function and also the elements $\varepsilon = \operatorname{sign} x$ in the one-dimensional case and $r = \sqrt{\mathbf{x}^2}$ in the three-dimensional. The construction of these algebras became the solution of a nontrivial mathematical problem. The definition of the multiplication of generalized functions encounters many difficulties. In particular, it is impossible to retain many of the familiar properties of multiplication. Schwartz's well-known example[19] precludes associativity in an algebra containing the functionals δ, x, $1/x \in D'(R^1)$. A great many studies have been made of the problem of multiplying generalized functions; in many of them, the problem of constructing an algebra was not posed at all, merely the products of some concrete pairs of functionals being specified (see, for example, Refs. 20 and 21). Such products are defined as a rule by the regularization of generalized functions by various ordinary functions, for which multiplication has a unique meaning.[20-24] In this case, the product frequently depends on the method of regularization that is employed. Sometimes multiplication is defined for all generalized functions in a particular class, though the products obtained in this way are in general not generalized functions by hyperdistributions, for which multiplication is not defined (see, for example, Ref. 24). Recently, the formalism of "nonstandard analysis" has been used to construct products of functionals.[25] Similar ideas were used in the construction of a theory of "asymptotic functions."[26]

Many studies use an approach that can be characterized as axiomatic. In it, one specifies in advance the properties that the algebra to be constructed must possess, and then multiplication is defined in the algebra without the use of regularization.[27-31] The method used in Shirokov's studies is also axiomatic. The requirements on the algebra follow directly from physical properties and, taken together, form a nontrivial system of axioms that in practice uniquely determine the algebra. One of the main requirements is associativity, which corresponds to the associativity of the algebra of observables of quantum theory. Another important requirement, which also has a physical origin, is the existence of an operation of differentiation. In addition, it must be possible not only to multiply the elements of the algebra with one another but also to multiply by the quantities that describe the state vectors of the physical system. In the algebra there must also be defined a bilinear form, which is necessary for defining quantum-mechanical expectation values. On the other hand, it has proved necessary to give up other familiar but physically unimportant requirements. Thus the algebras constructed in Refs. 1 and 2 are not commutative ($\delta\varepsilon = -\varepsilon\delta$ in the one-dimensional and $\delta r = -r\delta$ in the three-dimensional case), and the elements of the algebras are of necessity not the "ordinary" generalized functions of the spaces D' or S' but functionals on a space of test functions that themselves can have singularities of a definite type at the origin.

The review of Refs. 1–9 presented below divides naturally into two parts, the first of which contains the mathematical formalism of associative algebras of generalized functions, and the second its application in quantum-mechanical problems with δ-functional potentials. In the first part, we begin by constructing the algebras in the one-dimensional (Sec. 1) and three-dimensional (Sec. 2) cases. Section 3 describes the construction of an algebra closed with respect to the operations of differentiation and the taking of the antiderivative. In the second part, in Sec. 4, a method is formulated for solving problems with δ-functional potentials; it is illustated and made more precise on the basis of examples in the one-dimensional case. In Sec. 5, the method is used to solve the simplest three-dimensional problems. This section also considers physically nontrivial problems of motion in the field of a δ-functional potential in the p state and the interaction of a charged quantum-mechanical particle with the electromagnetic field in the presence of a strongly singular potential. Finally, in Sec. 6 the construction of a representation of free solutions for the Schrödinger equation with strongly singular potentials is described.

1. ASSOCIATIVE ALGEBRA OF GENERALIZED FUNCTIONS IN THE ONE-DIMENSIONAL CASE

The associative algebra $\mathcal{A}$ of generalized functions with differentiation and involution constructed in Ref. 1 and intended for the description of δ-functional quantum-mechanical potentials has the following properties.

1. For $x \neq 0$, the elements of $\mathcal{A}$ are infinitely differentiable functions.

2. On $\mathcal{A}$ there is defined an associative operation of multiplication: $A, B \to AB$, this being identical to ordinary multiplication whenever the elements of the algebra are ordinary functions, i.e., at least for $x \neq 0$.

3. On $\mathcal{A}$ and $\Psi (\Psi \subset \mathcal{A}$ is the subspace characterized by rapid decrease of the elements $\psi(x) \in \Psi$ as $|x| \to \infty$) there is defined a bilinear functional $\langle A, \psi \rangle$, and

$$\langle A B, \psi \rangle = \langle A, B\psi \rangle, A, B \in \mathcal{A}, \psi \in \Psi. \tag{1}$$

4. On $\mathcal{A}$ there is defined the operation of differentiation $\partial = d/dx$, which is identical to ordinary differentiation whenever the elements of the algebra are differentiable functions. The Leibnitz rule holds:

$$\frac{d}{dx}(AB) = \frac{dA}{dx} B + A \frac{dB}{dx}, \tag{2}$$

and also the relation

$$\left\langle \frac{dA}{dx}, \psi \right\rangle = -\left\langle A, \frac{d\psi}{dx} \right\rangle \tag{3}$$

for all $A, B \in \mathcal{A}$, $\psi \in \Psi$.

5. On $\mathcal{A}$ there is defined the involution operation $f \to f^*$, which is identical to complex conjugation in the region in which the elements of the algebra are ordinary functions; it commutes with differentiation and satisfies the relation

$$\langle f, g \rangle^* = \langle g^*, f^* \rangle \tag{4}$$

(the asterisk denotes the complex conjugate).

It follows from the listed properties that $\mathcal{A}$ cannot be realized on some subset of ordinary generalized functions $D'(R)$ or $S'(R)$. Its elements are functionals over the space Ψ_f of test functions that for $x \neq 0$ behave as functions in $S(R)$: They are infinitely differentiable, and as $x \to \pm\infty$ decrease faster than $|x|^{-n}$ for any $n > 0$. In addition, at the origin there exist the limits $\psi^{(n)}(\pm 0)$ from the right and the left of all the derivatives $\psi^{(n)}(x)$. It is convenient to introduce the notation

$$\psi_s^n = (\psi^{(n)}(+0) + \psi^{(n)}(-0))/2;$$
$$\psi_a^n = (\psi^{(n)}(+0) - \psi^{(n)}(-0))/2.$$

The space $\mathcal{A}_f$ (it forms a subalgebra of $\mathcal{A}$) consists by definition of functions which differ from $\psi \in \Psi_f$ only by the behavior at infinity: They are polynomially bounded together with all their derivatives. On $\mathcal{A}_f$ and Ψ_f the following bilinear functional is naturally defined:

$$\langle A, \psi \rangle = \int dx A(x) \psi(x), \quad A \in \mathcal{A}_f, \quad \psi \in \Psi_f. \tag{5}$$

Any element of $\mathcal{A}_f$ defines in accordance with (5) a linear functional on Ψ_f. In addition, on Ψ_f for $n = 0, 1, 2, \ldots$ there are defined the functionals $\delta_s^{(n)}$ and $\delta_a^{(n)}$ ($\delta_{s(a)}^{(0)} = \delta_{s(a)}$):

$$\langle \delta_s^{(n)}, \psi \rangle = (-1)^n \psi_s^{(n)}; \tag{6}$$
$$\langle \delta_a^{(n)}, \psi \rangle = (-1)^n \psi_a^{(n)}, \tag{7}$$

whose support is concentrated at the point $x = 0$ (the concept of support can be readily generalized to the case of the space Ψ_f').

By definition,[1] an arbitrary element of $\mathcal{A}$ has the form

$$A(x) = A_f(x) + \sum_{m=0}^{M(A)} A_m \delta_s^{(m)}(x) + \sum_{n=0}^{N(A)} A^n \delta_a^{(n)}(x) \equiv A_f(x) + A_{\text{sing}}(x);$$
$$A_f \in \mathcal{A}_f, \quad A_m, \quad A^n \in C. \tag{8}$$

Thus, $A \in \mathcal{A}$ is defined by a function $A_f(x) \in A_f$ and two terminating sequences $\{A_1, \ldots, A_{M(A)}\}$ and $\{A^1, \ldots, A^{N(A)}\}$. An arbitrary element of the subalgebra $\Psi \subset \mathcal{A}$, which is intended for the description of the state vectors, can be represented in the form

$$\psi(x) = \psi_f(x) + \sum_{m=0}^{M(\psi)} \psi_m \delta_s^{(m)}(x) + \sum_{n=0}^{N(\psi)} \psi^n \delta_a^{(n)}(x) \equiv \psi_f(x) + \psi_{\text{sing}}(x);$$
$$\psi_f \in \Psi_f, \quad \psi_m, \quad \psi^n \in C. \tag{9}$$

For $A \in \mathcal{A}_f$, $\psi \in \Psi_f$ the expression for the bilinear functional reduces to (5). In the general case, it is determined by

$$\langle A, \psi \rangle = \langle A_f, \psi_f \rangle + \langle A_{\text{sing}}, \psi_f \rangle - \langle \bar{\psi}_{\text{sing}}, \xi A_f \rangle, \tag{10}$$

where $\bar{\psi}_{\text{sing}}$ differs from ψ_{sing} only by the sign in one of the terms [cf. Ref. 8]:

$$\bar{\psi}_{\text{sing}} = \sum_{m=0}^{M} \psi_m \delta_s^{(m)} - \sum_{n=0}^{N} \psi^n \delta_a^{(n)},$$

and $\xi \in D(R)$ is a function equal to unity in some neighborhood of the point $x = 0$. For brevity, the symbol $\langle , \rangle$ will denote both the bilinear functional on $\mathcal{A}$ and Ψ and the action of a functional of $\mathcal{A}$ on $\psi \in \Psi_f$, which should not lead to confusion.

For $x \neq 0$, differentiation of elements of $\mathcal{A}$ is identical to ordinary differentiation. For "singular" elements, it is given by the relations

$$\partial \delta_s^{(n)} = \delta_s^{(n+1)}, \quad \partial \delta_a^{(n)} = \delta_a^{(n+1)}. \tag{11}$$

Finally, since any function $A(x) \in \mathcal{A}_f$ admits the representation

$$A(x) = A_1(x) + \varepsilon(x) A_2(x), \quad A_{1,2} \in \mathcal{A}_f \cap C^\infty, \quad \varepsilon(x) = \text{sign } x,$$

it is also necessary to specify differentiation of the element $\varepsilon(x)$:

$$\partial \varepsilon = 2\delta_s. \tag{12}$$

This equation is rather natural, since it is satisfied on restriction to $S(R) \subset \Psi_f$. At the same time, $\delta_s^{(n)}$ acts on $\psi \in S(R)$ as the n-th derivative of the ordinary δ function, so that in what follows we use instead of $\delta_s^{(n)}$ the symbol $\delta^{(n)}$. It is easy to show that the rules of differentiation that we have formulated ensure fulfillment of the property expressed by Eq. (3).

Multiplication is introdcued in the algebra as follows. The product of functions in $\mathcal{A}_f$ is identical to the ordinary product. The product of any two δ-functional elements is by definition equal to zero:

$$\delta^{(n)} \delta^{(m)} = 0. \tag{13}$$

Products of the type $\delta^{(n)} A$ and $\delta_a^{(n)} A$ for $A \in A_f$ are defined to ensure fulfillment of property 2 [Eq. (1)]. In particular, it follows from this requirement that

$$\delta^{(n)} \varepsilon = \delta_a^{(n)}, \tag{14}$$

which can be used to denote $\delta_a^{(n)}$. Similarly, we can establish the relations

$$\delta^{(n)} x^m = \begin{cases} \frac{(-1)^m n!}{(n-m)!} \delta^{(n-m)}, & n \geqslant m, \\ 0, & n < m. \end{cases} \tag{15}$$

Finally, it remains to define products of the type $A\delta^{(n)}$ for $A \in \mathcal{A}_f$. In the case $A \in \mathcal{A}_f \cap C^\infty$ the elements $A(x)$ commute with $\delta^{(n)}$:

$$A\delta^{(n)} = \delta^{(n)} A.$$

However, the element $\varepsilon(x)$ cannot commute with $\delta^{(n)}$. It follows from the requirement of fulfillment of Leibnitz's rule and the relation (12) that

$$(\varepsilon\varepsilon)' = 1' = 0 = 2(\delta\varepsilon + \varepsilon\delta),$$

from which it follows that ε and δ must anticommute:

$$\varepsilon\delta = -\delta\varepsilon. \tag{16}$$

After $(n-1)$-fold differentiation of this equation using (13), we obtain the more general rule of multiplication

$$\varepsilon\delta^{(n)} = -\delta^{(n)}\varepsilon. \tag{17}$$

It is easy to show that the algebra is associative and that Leibnitz's rule is satisfied.

The involution operation, which satisfies the standard requirements $(A^+)^+ = A$, $(\lambda A)^+ = \lambda^* A^+$, $(AB)^+ = B^+ A^+$ for $A, B \in \mathcal{A}$, $\lambda \in C$, is identical to complex conjugation for ordinary functions $A \in \mathcal{A}_f$. The involution of singular elements is defined by

$$(\delta^{(n)})^+ = \delta^{(n)}. \tag{18}$$

It follows in particular from these rules that

$$(\varepsilon\delta^{(n)})^+ = \delta^{(n)}\varepsilon = -\varepsilon\delta^{(n)}.$$

It can be readily verified directly that the operations of differentiation and involution commute.

By means of the involution on Ψ and the bilinear functional one can define the sesquilinear form

$$\chi, \psi \to C: \quad (\chi, \psi) = \langle \chi^+, \psi \rangle.$$

The form $(,)$ is real ($\mathrm{Im}\langle \psi^+ \psi \rangle = 0$ for any $\psi \in \Psi$) but not positive definite; in particular,

$$(\delta, \delta) = 0.$$

2. ASSOCIATIVE ALGEBRA OF GENERALIZED FUNCTIONS IN THE THREE-DIMENSIONAL CASE

In Ref. 2, Shirokov constructed an algebra of generalized functions that is a three-dimensional analog of the algebra $\mathcal{A}$ and will be denoted by $\mathcal{A}_3$. For $\mathcal{A}_3$, the requirements expressed in properties 1–5 in Sec. 1 are generalized to the three-dimensional case and reformulated in equivalent form. Instead of the bilinear functional $\langle A, \psi \rangle$ a linear functional $\langle \psi \rangle$, called a renormalized integral and denoted by $\int d\mathbf{x}\psi(\mathbf{x})$, was used. Property 4, expressed by Eq. (3), is then replaced by the vanishing of $\langle \partial\psi \rangle$ for any $\psi \in \Psi_3$ (Ψ_3 is the three-dimensional analog of the space Ψ), which in the language of the "renormalized integral" corresponds to the possibility of formal integration by parts:

$$\int d\mathbf{x}\,(\partial_i A(\mathbf{x}))\,\psi(\mathbf{x}) = -\int d\mathbf{x} A(\mathbf{x})\,\partial_i \psi(\mathbf{x}), \tag{19}$$

where $\partial_i = \partial/\partial x_i$, $\mathbf{x} = (x_1, x_2, x_3)$.

The equivalence of the formulations follows from the fact that, using the presence of the associative operation of multiplication, one can always construct from the bilinear functional a linear functional and vice versa:

$$\langle \psi \rangle = \langle 1, \psi \rangle, \ \langle A, \psi \rangle = \langle A\,\psi \rangle, \quad A \in \mathcal{A}_3, \psi \in \Psi_3. \tag{20}$$

In contrast to the one-dimensional case, the algebra $\mathcal{A}_3$ was not realized as an algebra of functionals in some space.[2] In addition, not all the identities for its elements were written down. Two restricting rules were formulated, these being valid for any associative algebra of generalized functions for elements that have inverses, for example, $\varepsilon(x)$ in the one-dimensional algebra and $r = |\mathbf{x}|$ in the three-dimensional. First, the product of such an element with any other nonzero element cannot be equal to zero (since otherwise associativity is lost—Schwartz's well-known example[19] is based on this, for example). Second, differentiation of the product of an element and its inverse ($\varepsilon\varepsilon^{-1}$, rr^{-1}) must give zero. No other connection between the elements of $\mathcal{A}_3$ was decided upon, which is not important since for applications in quantum mechanics it was found to be sufficient to take into account elements with a very small number of singular terms.[4,5,7,8]

The algebra $\mathcal{A}_3$ was constructed to describe concentrated, strongly singular potentials, and it therefore includes δ-functional elements, and also the element r, whose differentiation yields the δ function. Thus, the generators of $\mathcal{A}_3$ are: 1) infinitely differentiable functions $A_{sm}(\mathbf{x})$; 2) r; 3) $\delta(\mathbf{x})$. All the remaining elements of the algebra can be obtained from these generators by means of a finire number of operations of multiplication, addition, and differentiation. The relations of the algebra $\mathcal{A}_3$ are

$$r^l \partial^n \delta = (-1)^l \{\partial^l \delta\}\, r^l \neq 0; \tag{21}$$

$$x_i \partial^n \delta = (\partial^n \delta)\, x_i \neq 0; \tag{22}$$

$$(\partial^m \delta)\,(\partial^n \delta) = 0; \tag{23}$$

$$r^l r^k = r^{l+k}; \tag{24}$$

$$\partial_i r = x_i r^{-1} + 4\pi x_i r^2 \delta, \tag{25}$$

where $m, n = 0, 1, 2\ldots$; $l, k = 0, \pm 1, \pm 2, \ldots$; $i = 1, 2, 3$.

Together, these relations ensure fulfillment of the equations

$$\partial_i (r^2) = 2x_i, \ \partial_i (rr^{-1}) = (\partial_i r)\, r^{-1} + r\partial_i (r^{-1}) = 0.$$

In addition, it follows from then that

$$\Delta (r^{-1}) = -4\pi\delta + 4\pi\partial_i (x_i \delta).$$

The involution in the algebra $\mathcal{A}_3$ is specified as follows:

$$(A_{sm}(\mathbf{x}))^+ = A_{sm}(\mathbf{x}), \ (\partial^n \delta)^+ = \partial^n \delta, \ r^+ = r.$$

Hence and from (21) there follows, for example, the relation

$$(r\delta)^+ = \delta r = -r\delta.$$

For the following applications, it was found to be sufficient to write the general element of the algebra in the form

$$A(\mathbf{x}) = A_f(\mathbf{x}) + \sum_n \partial^n (r^{-2k} A_{skn}(\mathbf{x})\,\delta(\mathbf{x})) + \sum_n \partial^n (r^{-2l-1} A_{aln}(\mathbf{x})\,\delta(\mathbf{x})), \tag{26}$$

where k and l are certain integers; as $A_f(\mathbf{x})$ one chooses, as a rule, a function that can be represented in the form (see Refs. 4, 5, and 8)

$$A_f(\mathbf{x}) = A_s(\mathbf{x}) + r^{-1} A_a(\mathbf{x}).$$

Here and in (26), $A_{skn}(\mathbf{x})$, $A_{aln}(\mathbf{x})$, $A_s(\mathbf{x})$, $A_a(\mathbf{x})$ are infinitely differentiable functions, and A_{skn} and A_{aln} are defined only in an arbitrary neighborhood of the point $\mathbf{x} = 0$.

The general form of the renormalized integral $\int d\mathbf{x} A(\mathbf{x})$ is defined as follows [it is assumed that $A_f(\mathbf{x})$, which contributes to $A(\mathbf{x})$, is a function that is integrable at large r]. From the complete sum (26), contributions to the renormalized integral are made by only $A_f(\mathbf{x})$ and the term equal to a number multiplied by $\delta(\mathbf{x})$:

$$\int d\mathbf{x} A(\mathbf{x}) = \int d\mathbf{x} A_f(\mathbf{x}) + a_k (\Delta^k A_{sk0})(0), \tag{27}$$

where a_k is a combinatorial factor, determined by the form of the coefficient of r^{2k} in the expansion of $A_{sk0}(\mathbf{x})$ in a Maclaurin series, for example, $a_0 = 1$. One can show directly that for this definition of the renormalized integral the property expressed by Eq. (19) is satisfied.

It should be noted that in the constructed algebra $\mathcal{A}_3$ the element r is analogous to the element ε in $\mathcal{A}$. Both these elements anticommute with the δ function. The δ function can be obtained from both by means of dif-

ferentiations. Both elements have inverses, and therefore their product on any nonvanishing element of the algebra is not equal to zero.

The sesquilinear form by means of which the quantum-mechanical mean values are expressed is constructed from the linear functional $\langle\psi\rangle$ and the involution in a natural manner:

$$(\chi, \psi) = \langle\chi^+, \psi\rangle = \int dx\, \chi^+(x)\, \psi(x),$$

so that the expectation value of the operator $A(x)$, which is a linear combination of operators of multiplication by elements in $\mathcal{A}_3$ and operators of differentiation, can be written in the form

$$(\psi, A(x)\psi) = \int dx\, \psi^+(x)\, A(x)\, \psi(x).$$

It must be borne in mind that in the last two equations the integrals are understood as renormalized. As in the case of the algebra $\mathcal{A}$, the form (χ, ψ) is not positive definite, which follows, for example, from the nonpositivity of the functionals r^{-n} for $n \geq 3$: $\langle r^{-n}, \varphi\rangle$ may be negative for $\varphi \geq 0$.

3. ASSOCIATIVE ALGEBRA OF GENERALIZED FUNCTIONS CLOSED WITH RESPECT TO DIFFERENTIATION AND TAKING OF THE ANTIDERIVATIVE

In accordance with (10), any element of the algebra $\mathcal{A}$ defines a linear functional on the space Ψ, each of whose elements (9) is specified by a function $\psi_f(x)$ and two terminating sequences $\{\psi_1, \ldots, \psi_{M(\psi)}\}$ and $\{\psi^1, \ldots, \psi^{N(\psi)}\}$ (this was already noted above in connection with elements of $\mathcal{A}$). Besides such functionals on Ψ, one can, for example, define the functionals $\eta^{(n)}$ and $\eta^{(n)}\varepsilon$:

$$\langle\eta^{(n)}, \psi\rangle = \psi_n, \quad \langle\eta^{(n)}\varepsilon, \psi\rangle = \psi^n, \tag{28}$$

which have support at the origin and therefore can describe concentrated singular potentials. It is natural to pose the problem of constructing an algebra containing the algebra $\mathcal{A}$ and including the elements $\eta^{(n)}$. This problem was posed in Ref. 3 and solved in Ref. 6. In the solution of this problem, an algebra arises that is closed not only with respect to the operations introduced earlier but also with respect to the taking of the antiderivative. It should be noted that $\mathcal{A}$ does not have this property. In it, for example, there is no antiderivative of the element $\varepsilon\delta$, since the derivative of $\eta = \eta^{(0)}$ must be equal to $2\varepsilon\delta$ in accordance with property 4 [Eq. (3)].

The construction of an algebra containing $\varepsilon(x)$, $\delta^{(n)}(x)$, $\eta(x)$ is done axiomatically, without definition of the elements $\varepsilon, \delta, \eta$ as functionals on some space of test functions, as was done in the case of the algebra $\mathcal{A}$. This is achieved by separating the algebraic and functional aspects of the problem; namely, for the symbols $x, \varepsilon, \delta, \eta$, irrespective of how they are interpreted, axioms are formulated and on their basis the algebra $\mathfrak{A}$, in which $x, \varepsilon, \delta, \eta$ are generators, is constructed. Giving these symbols the meaning of functionals on some space of test functions, we can realize $\mathcal{A}$ as an algebra of generalized functions (see below).

The axioms that generalize properties 1–4 (see Sec. 1) and the necessary definitions have the following form: $\mathfrak{A}$ is a linear associative algebra with unit element over the field of complex numbers. The operation of differentiation ∂ on $\mathfrak{A}$ is defined by the relations

$$\left.\begin{array}{l} \partial x = 1, \quad \partial 1 = 0, \quad \partial\varepsilon = 2\delta, \quad \partial\delta = \delta^{(1)}, \quad \partial\delta^{(n)} = \delta^{(n+1)}, \\ \partial\eta = 2\varepsilon\delta, \quad \partial(fg) = (\partial f)\, g + f\, \partial g, \quad \partial\lambda f = \lambda\, \partial f, \\ \lambda \in C, \quad f, g \in \mathfrak{A}, \quad n = 1, 2, \ldots. \end{array}\right\} \tag{29}$$

The following identities are satisfied in $\mathfrak{A}$:

$$\left.\begin{array}{l} \varepsilon\varepsilon = 1, \quad x\delta = \delta x = 0, \quad \delta^{(m)}\delta^{(n)} = 0, \\ x\varepsilon = \varepsilon x, \quad \eta\varepsilon = -\varepsilon\eta, \quad \eta x = x\eta, \quad m, n = 0, 1, \ldots. \end{array}\right\} \tag{30}$$

The involution in the algebra $\mathfrak{A}$ is defined by

$$\left.\begin{array}{l} x^+ = x, \quad \varepsilon^+ = \varepsilon, \quad \delta^+ = \delta, \quad \eta^+ = -\eta, \\ (fg)^+ = g^+ f^+, \quad (f^+)^+ = f, \quad f, g \in \mathfrak{A}. \end{array}\right\} \tag{31}$$

The operation of involution commutes with differentiation:

$$(\partial f)^+ = \partial(f^+). \tag{32}$$

On the algebra $\mathfrak{A}$ the bilinear functional $\langle , \rangle$ is defined, and it is sufficient to define it only on the elements 1 and δ:

$$\langle 1, \delta\rangle = 1. \tag{33}$$

The axioms relating involution, differentiation, multiplication, and the functional have the form

$$\langle fg, h\rangle = \langle f, gh\rangle, \quad f, g, h \in \mathfrak{A}; \tag{34}$$

$$\langle f^+, g\rangle = \langle g^+, f\rangle^*. \tag{35}$$

To write down the axiom for integration by parts, the analog of the expression $f(x)g(x)\big|_{-a}^{a}$ is defined. For this, we introduce the functional $\big|_{-a}^{a}$:

$$\varepsilon\big|_{-a}^{a} = 2, \quad x^{2n+1}\big|_{-a}^{a} \neq 0, \quad x^{2n}\varepsilon\big|_{-a}^{a} \neq 0, \quad n = 0, 1, \ldots. \tag{36}$$

On the remaining elements of $\mathfrak{A}$ this functional gives zero. The asiom of integration by parts has the form

$$\langle\partial f, g\rangle = -\langle f, \partial g\rangle + fg\big|_{-a}^{a}. \tag{37}$$

For example, for 1 and δ the expression (37) is written as

$$1 = \langle 1, \delta\rangle = \tfrac{1}{2}\langle 1, \partial\varepsilon\rangle = \tfrac{1}{2}\varepsilon\big|_{-a}^{a} - \tfrac{1}{2}\langle 0, \varepsilon\rangle = 1.$$

THEOREM 1. Axioms (29)–(37) are satisfied by a unique algebra $\mathfrak{A}$, in which

$$\left.\begin{array}{l} \varepsilon\delta = -\delta\varepsilon, \quad \partial x^n = nx^{n-1}, \quad \eta'\eta = \eta\eta', \quad (\eta' = \partial\eta); \\ \eta\delta = -\delta\eta, \quad (\eta^p)' = p\eta'\eta^{p-1}, \quad p = 1, 2, \ldots; \\ \eta\delta^{(m)} = -\delta^{(m)}\eta, \quad (x^n\eta)' = nx^{n-1}\eta. \end{array}\right\} \tag{38}$$

For example, the last equation in (38) can be proved by means of the calculation

$$\begin{aligned} \partial^m(\eta\delta) &= \partial^{m-1}\partial(\eta\delta) = \partial^{m-1}(\eta'\delta + \eta\delta') \\ &= \partial^{m-1}\eta\delta' = \ldots = \eta\delta^{(m)}. \end{aligned}$$

At the same time, $\partial^m(\eta\delta) = -\partial^m(\delta\eta) = -\delta^{(m)}\eta$, which is what we had to prove.

Theorem 1 takes it possible to obtain the functional on all elements of the algebra $\mathfrak{A}$ from the axioms (29)–(31).

THEOREM 2.

$$\left.\begin{aligned}&\langle 1, x^n\rangle = \frac{1}{n+1}\, x^{n+1}\,|_{-a}^{a}, \quad \langle \varepsilon, \eta^k\rangle = 0, \quad \langle \varepsilon, \delta\eta^k\rangle = 0,\\ &\langle \eta^k\delta\rangle = k!, \quad \langle \eta^m, 1\rangle = 0, \quad \langle x^n\eta^m\rangle = 0, \quad \langle \delta^{(k)}, \eta^p\rangle = 0 \quad (k \neq 0).\end{aligned}\right\} \tag{39}$$

Proof. From the chain of equations

$$\langle x^n, 1\rangle = \langle x^n, x'\rangle = x^{n+1}\,|_{-a}^{a} - \langle nx^{n-1}, x\rangle = x^{n+1}\,|_{-a}^{a} - n\langle x^n, 1\rangle$$

it follows that

$$\langle 1, x^n\rangle = \frac{1}{n+1}\, x^{n+1}\,|_{-a}^{a},$$

$$\langle \eta^k, \delta\rangle = \frac{1}{2}\langle \eta^k\varepsilon'\rangle = -\frac{1}{2}\langle k\eta^{k-1}\varepsilon\delta\varepsilon\rangle = k\langle \eta^{k-1}, \delta\rangle.$$

This recursive equation leads to $\langle \eta^k\delta\rangle = k!$. The remaining propositions of the theorem are proved similarly.[6] From Theorem 2, we readily conclude that each of the elements of the form

$$x^m\eta^n, \ \delta^{(m)}\eta^n, \ \varepsilon x^m\eta^n, \ \varepsilon\delta^{(m)}\eta^n \tag{40}$$

is nonzero, since for all m, $n = 0, 1, 2, \ldots$ there exists an element $f \in \mathfrak{A}$ such that $\langle f, g\rangle \neq 0$, where g is one of the elements (40). It can be shown that the elements (40) are not only nonzero but also linearly independent, and the set of elements of the algebra $\mathfrak{A}$ is exhausted by linear combinations of them (for the proof, see Ref. 6).

The constructed algebra of formal symbols $x, \varepsilon, \delta, \eta$ can be realized as an algebra of functionals on the space of test functions represented in the form

$$\psi = \sum_n (\psi_{sn}(x) + \varepsilon(x)\,\psi_{an}(x)\,\eta^n(x)) + \sum_{m,\,n} (\psi_{mn}\delta^{(m)}\eta^n(x) + \varepsilon(x)\,\psi^{mn}\delta^{(m)}\eta^n(x)), \quad \psi_{sn}, \ \psi_{an} \in S(R^1). \tag{41}$$

Of course, the quantities $\delta^{(m)}$ and η^n in this expression are not functions, so that Eq. (41) is to be understood as the formal expression of the fact that an arbitrary element of the space of test functions is defined by a collection of functions and terminating sequences $(\{\psi_{sn}\}, \{\psi_{an}\}, \{\psi_{mn}\}, \{\psi^{mn}\})$ (see the analogous remarks with regard to the space Ψ in Sec. 1).

The relations (29)–(39) are valid in the algebra with the generators x, $\varepsilon(x)$, $\delta(x)$, $\eta(x)$, and the algebra $\mathcal{A}$ with generators x, ε, δ is a subalgebra of it. These relations show that together with every element the algebra $\mathfrak{A}$ contains all its derivatives and all its antiderivatives, i.e., the algebra is closed with respect to these operations.

4. APPLICATION OF ASSOCIATIVE ALGEBRAS OF GENERALIZED FUNCTIONS TO THE CONSTRUCTION OF ONE-DIMENSIONAL QUANTUM-MECHANICAL MODELS WITH SINGULAR POTENTIALS

The algebras of generalized functions $\mathcal{A}, \mathfrak{A}, \mathcal{A}_3$ considered in Secs. 1–3 can be used to describe strongly singular concentrated interactions in quantum mechanics. In this section, we give a general method for constructing dynamical schemes corresponding to singular concentrated interactions; it applies to the motion of a quantum-mechanical particle on a straight line.

To construct the algebra $\mathcal{U}$ of observables of quantum theory with singular potentials, each of the algebras $\mathcal{A}, \mathfrak{A}, \mathcal{A}_3$ must be completed by an operator of differentiation, corresponding, as usual, to the momentum operator. However, not all local observables can be obtained by such a completion. The point is that by definition an observable is local if for its corresponding operator A

$$\operatorname{supp} A\psi \subset \operatorname{supp} \psi$$

for all $\psi \in \Psi$.

In the case of the algebra $\mathcal{A}$ considered here, this condition is satisfied by the following operators, which will be needed subsequently:

$$\left.\begin{aligned}&B_{mn}\psi(x) = \delta^{(m)}(x)\,\psi_s^{(n)}, \quad B^{mn}\psi(x) = \varepsilon(x)\,\delta^{m}(x)\,\psi_a^{(n)};\\ &B_{,n}^{m}\psi(x) = \varepsilon(x)\,\delta^{m}(x)\,\psi_s^{(n)}, \quad B_{m}^{,n}\psi(x) = \delta^{(m)}(x)\,\psi_a^{(n)},\end{aligned}\right\} \tag{42}$$

where $\psi(x)$ is given by the expression (9), and it is also satisfied by the operators

$$D_{mn}\psi(x) = \delta^{(m)}(x)\,\psi_n, \ D^{mn}\psi(x) = \varepsilon(x)\,\delta^{(m)}(x)\,\psi^{(n)},$$
$$D_{,n}^{m}\psi(x) = \varepsilon(x)\,\delta^{m}(x)\,\psi_n, \ D_{m}^{,n}\psi(x) = \delta^{(m)}\psi^{(n)}.$$

The operators B can be expressed in terms of the elements of $\mathcal{A}$, for exanple,

$$B_{mn}\psi = \delta^{(m)}(x)\,(-1)^n\,\langle \delta^{(n)}(x), \psi, (x)\rangle, \tag{43}$$

which makes it possible to include B in the algebra $\mathcal{U}$.

For the operators D an expression analogous to (43) holds if a functional $\eta \in \mathfrak{A}$ is used; however, the operators D cannot be expressed in terms of the elements of the algebra $\mathcal{A}$. This has the consequences that involution is not defined for the operators D, and therefore they cannot be included in the algebra of local observables $\mathcal{U}$.

The algebra $\mathcal{U}$ is an algebra of observables of an indefinite quantum mechanics, since, as we have already noted in Sec. 3, the sesquilinear form defined on the space Ψ does not satisfy thecondition of positive definiteness. To give the theory a direct physical meaning, it is necessary to go over to subspaces of Ψ with positive metric and to subalgebras of the algebra of observables $\mathcal{U}$ invariant with respect to these subspaces.

The method of arriving at subspaces with definite metric on which Hamiltonians with singular concentrated potentials are defined consists of three stages, the details of which depend on the dimension of the configuration space and in the case of the algebra $\mathcal{A}$ have the following form. The first stage consists of transition from the space $\Psi(9)$ to one of the subspaces Ψ^{MN}, where $M, N = f, 0, 1, \ldots$. The values $M = f$, $N = f$ correspond to the absence in $\psi(x)$ of singular terms of the given type, and $M \neq f$, $N \neq f$ indicate the maximally admissible derivative of the δ function in the sum (9). For example, Ψ^{0f} and Ψ^{ff} consist of elements of the form

$$\psi(x) = \psi_f(x) + \delta(x)\,\psi_0; \tag{44}$$

$$\psi(x) = \psi_s(x) + \varepsilon(x)\,\psi_a(x) = \psi_f(x) \tag{45}$$

respectively.

The second stage consists of the transition from the spaces Ψ^{MN} to their subspaces with positive-definite metric. For this transition, it is sufficient to express the coefficients ψ_m and ψ^m on (9) in terms of linear combinations of the values of the derivatives $\psi_s^{(n)}(0)$ and $\psi_a^{(n)}(0)$:

$$\left.\begin{aligned}\psi_m &= \sum_{n=0}^{M} b^{mn}\psi_s^{(n)} + \sum_{n=0}^{N} b^m_{,n}\psi_a^{(n)};\\ \psi^m &= \sum_{n=0}^{M} b^{,n}_{m}\psi_s^{(n)} + \sum_{n=0}^{N} b_{mn}\psi_a^{(n)}.\end{aligned}\right\} \tag{46}$$

When the conditions (46) are imposed, the sesquilinear form (χ, ψ) is positive definite on vectors in Ψ^{MN} if

$$\left.\begin{aligned}&b^{nn} = (-1)^n g_{sn} + ih_{sn}, \quad b_{nn} = (-1)^n g_{an} + ih_{an};\\ &g_{sn} \geqslant 0, \quad g_{an} \geqslant 0, \quad h^*_{sn} = h_{sn}, \quad h^*_{an} = h_{an};\\ &b^*_{mn} = -b_{nm}(-1)^{n-m}, \quad m \neq n;\\ &b^{mn*} = -b^{nm}(-1)^{n-m}, \quad b^m_{,n} = -b^{m*}_{n}(-1)^{n-m}.\end{aligned}\right\} \tag{47}$$

We denote the obtained subspace with definite metric by Ψ^{MN}_+. It is readily seen that the algebra of observables $\mathcal{U}$ does not leave the set Ψ^{MN}_+ invariant. Thus, the operator of differentiation carries the elements out of this set for all M, N. The algebra of local observables for the space Ψ^{MN}_+, denoted by $\mathcal{U}^{MN}_+$, can be obtained by using the independent operators P_f, $P_{MN} \in \mathcal{U}$ defined by

$$P_f\psi = \psi_f; \tag{48}$$

$$P_{MN}\psi = \Big(\sum_{m=0}^{M}\sum_{n=0}^{M} B_{mn}b^{mn} + \sum_{m=0}^{M}\sum_{n=0}^{N} B^n_m b^m_{,n} - \sum_{m=0}^{N}\sum_{n=0}^{M} B^m_{,n} b^n_m + \sum_{m=0}^{N}\sum_{n=0}^{N} B^{mn} b_{mn}\Big)\psi. \tag{49}$$

By direct calculation it is readily shown that $(P_f + P_{MN})\psi \in \Psi^{MN}_+$ for any $\psi(x) \in \Psi$. By definition, the algebra $\mathcal{U}^{MN}_+$ is the right deal of the algebra $\mathcal{U}$ generated by the idempotent $P_f + P_{MN}$ and, as one can show, is exhausted by polynomials in the operators $A_f + \Delta_{MN}$ and $d/dx + d_{MN}$, which are defined by the relations

$$(A_f + \Delta_{MN})\psi = P_f(A_f\psi) + P_{MN}(A_f\psi); \tag{50}$$

$$(d/dx - d_{MN})\psi = P_f(d\psi/dx) + P_{MN}(d\psi/dx). \tag{51}$$

It should be noted that $\mathcal{U}^{MN}_+$ is not invariant with respect to involution.

The third stage consists of choosing the candidate for the part of the Hamiltonian L and the additional restriction of the space Ψ^{MN}_+ to the space Ψ^{MN}_L, on which the corresponding operator L is symmetric. It is convenient to split this stage into several successive steps.

A. We choose an operator $L \in \mathcal{U}^{MN}_+$ whose expectation value has an imaginary part that depends only on $\psi_s^{(n)}(0)$, $\psi_a^{(n)}(0)$, $\psi_s^{(n)*}(0)$, $\psi_a^{(n)*}(0)$.

B. The imaginary part of the expectation value of L is equated to zero:

$$(\psi, L\psi) - (\psi, L\psi)^* = 0. \tag{52}$$

In accordance with the requirement imposed on L, the left-hand side of (52) is a bilinear form in $\psi_s^{(n)}$, $\psi_a^{(n)}$ and $\psi_s^{(n)*}$, $\psi_a^{(n)*}$.

C. The quantities $\psi_a^{(n)}$ in (52) are equated to linear combinations of $\psi_s^{(n)}$ with undetermined coefficients:

$$\psi_a^{(m)} = \sum a_{mn}\psi_s^{(n)}. \tag{53}$$

The indices m and n take all the values for which they are present in (52).

D. When (53) is substituted in (52), a system of equations for the coefficients a_{mn} is obtained. To each nontrivial solution of this system there corresponds the subspace Ψ^{MN}_L of the space Ψ^{MN}_+ on which the operator L is symmetric. Thus, some of the operators L can be chosen as Hamiltonians of nontrivial models with singular potentials.

This scheme must be augmented by the following considerations. The completion of the set Ψ^{MN}_+ with respect to the sesquilinear form on it leads to a Hilbert space $\mathcal{H}$ having the structure of a direct sum of spaces: $\mathcal{H} = L_2 \oplus C^1 \oplus \ldots \oplus C^1$. The closure of the operator L with domain of definition Ψ^{MN}_L in the space $\mathcal{H}$ leads to a self-adjoint Hamiltonian on $\mathcal{H}$. The Hamiltonians obtained by this scheme are parametrized by the admissible sets of quantities of the type $\{b\}$ and $\{a\}$; inequivalent dynamical models do not always correspond to different sets of these quantities. The above method of constructing quantum models with singular potentials can be readily generalized to the three-dimensional case. The resulting models with singular potentials differ strongly from the models of ordinary quantum mechanics with regular potentials for the following reasons.

a) The Hamiltonians corresponding to them cannot be represented as sums of kinetic- and potential-energy operators. These last are not defined on the set Ψ^{MN}_L. Only the total operator L is defined.

b) In the general case, the Hamiltonians are realized on spaces that differ from spaces of square-integrable functions. Despite this, such models are entirely acceptable from both the physical and mathematical points of view. For them, the axioms of quantum theory are satisfied and there exists a sensible scattering theory, which can be formulated mathematically as scattering theory in a pair of spaces.[32]

The general scheme was used to construct specific one-dimensional models.[3]

Example 1. Particle in the field of a singular potential of the type $\delta(x)$:

$$\Psi^{MN}_+ = \Psi^{ff}_+. \tag{54}$$

In this case, the metric is positive, and the operators Δ_{ff}, d_{ff} in (50), (51) have the form

$$\Delta_{ff} = 0, \; d_{ff}\psi = -2\delta(x)\psi_a. \tag{55}$$

As the operator L we choose

$$H_{ff}\psi = -(d/dx + d_{ff})^2\psi. \tag{56}$$

The explicit action of this operator on the set Ψ^{ff}_+ can be described by

$$H_{ff}\psi_f(x) = -\psi_f''(x) + 2\delta(x)\psi_a' + 2\delta'(x)\psi_a. \tag{57}$$

The operator H_{ff} is not symmetric on Ψ^{ff}_+. For this operator, Eq. (53) can be written in the form

$$\psi_s^*\psi_a' - \psi_s'^*\psi_a - \psi_a'^*\psi_s + \psi_a^*\psi_s' = 0. \tag{58}$$

The relations (53) reduce to

$$\psi_a = a_{00}\psi_s + a_{01}\psi_s', \; \psi_a' = a_{10}\psi_s + a_{11}\psi_s' \tag{59}$$

and when they are substituted in (58) lead to conditions the coefficients $\{a\}$:

$$a_{11} = -a_{00}^*, \; a_{01} = a_{01}^*, \; a_{10} = a_{10}^*. \tag{60}$$

The operator H_{ff} is essentially self-adjoint on the set

Ψ_H^{ff} and can be parametrized by virtue of the relations (60) by four real parameters. The situation in which $a_{01}\neq 0$, $a_{10}=a_{00}=0$ corresponds to what is usually called the Schrödinger equation with potential $a_{01}\delta(x)$. This situation corresponds to the case of the subspace of even functions $\psi(x)=\psi(-x)$.

The solutions of the Schrödinger equation with the Hamiltonian (57) and boundary conditions (59) corresponding to scattering (i.e., reflection and transmission) of a plane wave number k will have the form

$$\left.\begin{aligned}\psi_f(x)&=e^{ikx}+A(k)\,e^{-ikx}, \quad x<0,\\ \psi_f(x)&=B(k)\,e^{ikx}, \quad x>0,\end{aligned}\right\} \tag{61}$$

where $A(k)$ and $B(k)$ are complex coefficients determined by the boundary conditions:

$$\left.\begin{aligned}A(k)&=D^{-1}(k)\,[a_{01}k^2-ik(a_{00}+a_{00}^*)+a_{10}];\\ B(k)&=D^{-1}(k)\,[a_{01}a_{10}-(1+a_{00})(1-a_{00}^*)];\\ D(k)&=a_{01}k^2+ik(a_{01}a_{10}+a_{00}a_{00}^*+1)-a_{10}.\end{aligned}\right\} \tag{62}$$

In this example, different physically inequivalent systems correspond to different state of parameters $\{a\}$. It can be seen from (62) that B vanishes for $a_{01}a_{10}-(1+a_{00})(1-a_{00}^*)=0$, i.e., irrespective of the momentum, complete reflection with a nontrivial change in the phase of the incident wave will be observed.

Up to a normalization factor, the vectors in Ψ_H^{ff} describing bound states have the form

$$\left.\begin{aligned}\psi_f(x)&=e^{\varkappa x} \quad \text{for} \quad x<0;\\ \psi_f(x)&=e^{-\varkappa x} \quad \text{for} \quad x>0,\end{aligned}\right\} \tag{63}$$

where the parameter $\varkappa$ is related to the binding energy E by $E=-\varkappa^2$ and is determined by the equation

$$a_{01}\varkappa^2+(1+a_{00}a_{00}^*+a_{10}a_{01})\,\varkappa+a_{10}=0. \tag{64}$$

It can be seen from this equation that the system may have one, two, ir no bound states at all. It should be noted that for complex a_{00} the constant C is complex, so that the state vector of the lowest nondegenerate level may be complex. For $a_{00}=0$, $a_{10}=a_{10}^{-1}<0$ there exist two levels, for which

$$\varkappa_1=\varkappa_2=-a_{10}. \tag{65}$$

The possibility of a degenerate ground level and complex state vectors for the ground level are unusual properties of the Hamiltonians H_{ff}. The considered model is realized in the ordinary Hilbert space L_2 of square-integrable functions. The following example gives a model of a different type.

Example 2. Particle in the field of a singular potential of the type $\delta''(x)$.

In this case $\Psi^{MN}=\Psi^{0f}$. The elements of the space Ψ^{0f} have the form $\psi=\psi_f(x)+\delta(x)\psi_1$. A general transformation to a positive-definite form is defined by the relation $\psi_1=b^{00}\psi_s=(g_{s0}+ih_{s0})\psi_s$, where $g_{s0}\geqslant 0$, $h_{s0}^*=h_{s0}$. The elements of the space Ψ_+^{0f} therefore have the form $\psi=\psi_f(x)+b^{00}\delta(x)\psi_f$ and the sesquilinear form $(\ldots)$ on the set of these elements is determined by the equation

$$(\chi,\psi)=\int dx\chi_f^*(x)\psi_f(x)+2g_{s0}\chi_s^*\psi_s. \tag{66}$$

Completion with respect to the form (66) leads to the Hilbert space $\mathcal{H}=L_2\oplus C^1$, which consists of pairs $\{h\}=\{h,H\}$, $h\in L_2$, $H\in C^1$ with the scalar product $(\{h\},\{h'\})=\int dx h^*(x)h'(x)+2g_{s0}H^*H'$.

In accordance with the rules (50) and (51), the operators Δ_{0f} and d_{0f} have the form

$$\left.\begin{aligned}\Delta_{0f}\psi(x)&=b^{00}\delta(x)\,A_a\psi_a-b^{00}\varepsilon(x)\,\delta(x)\,A_a\psi_s;\\ d_{0f}\psi(x)&=b^{00}\delta(x)\,\psi_s'-b^{00}\delta'(x)\,\psi_s-2\delta(x)\,\psi_a.\end{aligned}\right\} \tag{67}$$

As in Example 1, the Hamiltonian of the system is determined by $H_{0f}=-(d/dx+d_{0f})^2$, which in expanded form can be written as

$$\begin{aligned}H_{0f}\psi(x)=&-\psi''(x)-b^{00}\delta(x)\,\psi_s''+2\delta(x)\,\psi_a'\\&+2\delta'(x)\,\psi_a+b^{00}\delta''(x)\,\psi_s.\end{aligned} \tag{68}$$

Equation (53) for the operator $L=H_{0f}$ can be solved on substitution of the relations (54), which in the considered case have the form

$$\psi_a=a_{00}\psi_s+a_{01}\psi_s'+a_{02}\psi_s'',\ \psi_a'=a_{10}\psi_s+a_{11}\psi_s'+a_{12}\psi_s''. \tag{69}$$

The solutions are determined by the set of parameters $\{a\}$ with the conditions

$$\left.\begin{aligned}&a_{02}=0, \quad a_{12}=\tfrac{1}{2}(b^{00}+b^{00*})=g_{s0};\\ &a_{10}=a_{10}^*, \quad a_{01}=a_{01}^*, \quad a_{11}=-a_{00}^*.\end{aligned}\right\} \tag{70}$$

The Hamiltonian H_{0f} is essentially self-adjoint on the set Ψ_H^{0f} as an operator on the space $\mathcal{H}$ and can be parametrized by the quantities g_{s0}, a_{00}, a_{10}, a_{01}.

The solutions of the Schrödinger equation corresponding to scattering are specified by the relations (61), in which the coefficients $A(k)$ and $B(k)$ can be expressed in accordance with (62) with the substitution $a_{10}\to a_{10}-k^2g_{s0}$. The equation for the bound states is an equation of the third degree in $\varkappa$:

$$a_{01}\varkappa^2+(1+a_{00}a_{00}^*+a_{01}a_{10}+a_{01}g_{s0}\varkappa^2)\,\varkappa+a_{10}-g_{s0}\varkappa^2=0. \tag{71}$$

Therefore, there are three bound states in the general case. Some of them may be on the unphysical sheet with respect to the energy. It follows from the expressions that we have written down that g_{s0} influences the physics of the model, but h_{s0} does not.

In the light of the approach we have presented, it is of interest to consider simultaneously regular and singular potentials.

Example 3. Harmonic oscillator in the field of a singular potential concentrated at a point.[9]

Let Ψ_H^{0f} be the set from Example 2. On this set, there is also defined the operator

$$H_{0f}=-(d/dx+d_{0f})^2+x^2/4, \tag{72}$$

which is the Hamiltonian of the considered system. It is necessary to find its eigenfunctions and eigenvalues. The solution is sought in the form

$$\left.\begin{aligned}\psi(x)&=D_\nu(-x), \quad x<0;\\ \psi(x)&=A_\nu D_\nu(x), \quad x>0, \ \nu=E-1/2.\end{aligned}\right\} \tag{73}$$

Here, A_ν is a constant, and $D_\nu(x)$ is a parabolic-cylinder function,[33] which satisfies the Schrödinger equation for the harmonic oscillator with $E=\nu+\frac{1}{2}$. Substitution of the functions (73) in the boundary conditions (69) and (70) gives the equation for the spectrum

$$[a_{10}-g_{s0}(\nu+1/2)]/\Gamma^2(1/2-\nu/2)$$
$$+[1+a_{10}a_{01}+a_{00}a_{00}^*-g_{s0}a_{01}(\nu+1/2)]\sqrt{2}/\Gamma(1/2-\nu/2)\,\Gamma(-\nu/2) \quad (74)$$
$$+2a_{01}/\Gamma^2(-\nu/2)=0,$$

where $\Gamma(\nu)$ is the gamma function. For the constant A_ν, we obtain the expression

$$A_\nu=1-2a_{00}\left(1+a_{00}+\sqrt{2}\,a_{01}\frac{\Gamma(1/2-\nu/2)}{\Gamma(-\nu/2)}\right)^{-1}. \quad (75)$$

For $a_{10}=g_{s0}=0$, the set of values $\nu=2k$, $k=0,1,2,\ldots$ is a solution of Eq. (74); for $a_{01}=0$, the set $\nu=2k+1$ is. Both these cases correspond to the levels and eigenfunctions of the unperturbed oscillator.

In the general case, we can calculate the small corrections to the levels of the harmonic oscillator due to the singularity, assuming $\nu=n+\alpha$, $|\alpha|\ll 1$. For the ground state, the correction has the form

$$\alpha_0=(2a_{10}-g_{s0})\left[2g_{s0}+\sqrt{\frac{\pi}{2}}(2+2a_{00}a_{00}^*+2a_{10}a_{01}-g_{s0}a_{01})\right. \quad (76)$$
$$\left.-(g_{s0}-2a_{10})(C+2\ln 2)\right].$$

Thus, by means of the developed method it is possible to construct a diverse family of single-particle Hamiltonian operators with singular potentials concentrated at a point. However, not all Hamiltonians with singular potentials can be included in the scheme; for example, ones with potential $a\delta'(x)$ cannot.

5. APPLICATION OF ASSOCIATIVE ALGEBRAS OF GENERALIZED FUNCTIONS TO THE CONSTRUCTION OF THREE-DIMENSIONAL MODELS WITH SINGULAR POTENTIALS

The general scheme for constructing models with singular potentials presented in the previous section for the example of one-dimensional case can be directly generalized to the three-dimensional case. The Hamiltonians are constructed in several Hilbert spaces successively in three stages. In the three-dimensional case, the method of Sec. 4 leads to a number of nontrivial models with singular concentrated potentials.

Example 1. Particle in the field of a potential of the type $\delta(x)$. The initial space Ψ^f is a subset of the space $L_2(R^3)$. The elements Ψ^f have the form

$$\psi_f(\mathbf{x})=\psi_s(\mathbf{x})-r^{-1}\psi_a(\mathbf{x}),\ r=|\mathbf{x}|, \quad (77)$$

where $\psi_s(\mathbf{x})$ and $\psi_a(\mathbf{x})$ are smooth functions that decrease at infinity. The sesquilinear form on Ψ^f is positive definite. In the three dimensional case, it is not possible to define operators ∂_i+d_{iQ} invariant with respect to Ψ_+^Q (Q is a multiple index that replaces the indices M and N in the one-dimensional case). However, requiring

$$\psi_a(\mathbf{x})=\varphi(r^2),\ \varphi(\xi)\in C^\infty(R^3), \quad (78)$$

we can construct the invariant operator H_f:

$$H_f\psi_f=-\Delta\psi_f(\mathbf{x})-4\pi\delta(\mathbf{x})\psi_a+$$
$$+8\pi x_i\delta(\mathbf{x})\partial_i\psi_a+4\pi\partial_i(x_i\delta(\mathbf{x}))\psi_a. \quad (79)$$

In accordance with the third stage of the general method, we impose on the set Ψ^f the condition (53) with $L=H_f$, i.e., $\mathrm{Im}(\psi,H_f\psi)=0$. By means of the explicit form of the elements of the space $\Psi^f(77)$ and the operator H_f (79) this condition can be simplified to

$$\psi_s^*(0)\psi_a(0)-\psi_a^*(0)\psi_s(0)=0, \quad (80)$$

whose solution is

$$\psi_a(0)=\alpha_0\psi_s(0),\ \alpha_0=\alpha_a^*. \quad (81)$$

Thus, we have obtained a one-parameter family of symmetric operators H_f on the subspaces $\Psi^f_{H_f}$ distinguished by the boundary condition (81). The closure of these operators in $L_2(R^3)$ gives a family of self-adjoint operators.

Example 1 is equivalent to what is usually called the Schrödinger equation with the potential $c\delta(\mathbf{x})$. This equation is treated from the point of view of extension of the operator $-\Delta$ from the subset of functions that vanish at $\mathbf{x}=0$ in Ref. 10. Such extensions are equivalent to extensions of the operator $-d^2/dr^2$ at the origin to the half-axis $(0,+\infty)$ and therefore lead to nontrivial scattering only for the s wave. This explains the reduction of the parameters compared with the case $(-\infty,\infty)$ of Example 1 in Sec. 4. The generalization of Example 2 in Sec. 4 to the three-dimensional case is the following example.

Example 2. Particle in the field of a potential of the type $\Delta\delta(\mathbf{x})$. The original space is Ψ^0. By definition, the elements of this space can be represented in the form

$$\psi=\psi_f(\mathbf{x})+\delta(\mathbf{x})\psi_0,\quad \psi_0\in C^1, \quad (82)$$

where $\psi_f(\mathbf{x})$ admits the representation (77). A sesquilinear form is defined on Ψ^0 by the rule

$$(\chi,\psi)=\int d\mathbf{x}\chi_f^*(\mathbf{x})\psi_f(\mathbf{x})-\chi_s^*(0)\psi_0-\chi_0^*\psi_s(0). \quad (83)$$

The transition to the subspace with a definite form is made by imposing the condition $\psi_0=g\psi_s(0)$; then

$$(\chi,\psi)=\int d\mathbf{x}\chi_f^*(\mathbf{x})\psi_f(\mathbf{x})+2g\chi_s^*(0)\psi_s(0). \quad (84)$$

The completion of Ψ_+^0 with respect to the form (84) generates the Hilbert space $\mathscr{H}=L_2(R^3)\oplus C^1$. As the Hamiltonian H invariant with respect to Ψ_+^0 we choose the operator

$$H\psi=-\Delta\psi(\mathbf{x})-4\pi\delta(\mathbf{x})\psi_a+8\pi x_i\delta(\mathbf{x})\partial_i\psi_a$$
$$-4\pi\partial_i(x_i\delta(\mathbf{x}))\psi_a(\mathbf{x})+g\Delta\delta(\mathbf{x})\psi_s-g\delta(\mathbf{x})\Delta\psi_s. \quad (85)$$

The third stage consists of solving the equation

$$(\psi,H\psi)-(\psi,H\psi)^*=-4\pi(\psi_s^*\psi_a-\psi_a^*\psi_s)+$$
$$+g(\Delta\psi_s^*\psi_s-\psi_s^*\Delta\psi_s)=0. \quad (86)$$

The linear ansatz $\psi_a=\alpha_0\psi_s+\alpha_2\Delta\psi_s$ is a solution of (86) under the conditions

$$\alpha_0^*=\alpha_0; \quad (87)$$

$$\alpha_2=\alpha_{22}^*=-(2\pi)^{-1}g. \quad (88)$$

These conditions determine the subspace Ψ_H^0. The closure of the operator H with domain of definition Ψ_H^0 in the space $\mathscr{H}$ defines a self-adjoint operator, the Hamiltonian of the considered system. The family of Hamiltonians can be parametrized by the two real parameters α_0 and g.

The solution of the Schrödinger equation $(H-E)\psi=0$ corresponding to scattering with energy $E=k^2$ and phase shift δ_k has the form

$$\psi(\mathbf{x}) = (kr)^{-1}\sin kr\cos\delta_k + (kr)^{-1}\cos kr\sin\delta_k + g\delta(\mathbf{x})\cos\delta_k. \quad (89)$$

It follows from this that

$$\psi_s = \cos\delta_k,\ \Delta\psi_s = -k^2\cos\delta_k,\ \psi_a = \frac{1}{k}\sin\delta_k. \quad (90)$$

Substitution of (89) in the boundary conditions with allowance for (90) gives an expression for the phase shift: $\tan\delta_k = \alpha_0 k + gk^3/2\pi$. Since the phase shifts of waves with $l>0$ are equal to zero, the scattering is isotropic, and the total cross section is given by the expression

$$\sigma = \frac{4\pi}{k^2}\sin^2\delta_k = \frac{4\pi(\alpha_0+gk^2/2\pi)^2}{1+k^2(\alpha_0+gk^2/2\pi)^2}. \quad (91)$$

In the presence of a bound state with binding energy $E=-\varkappa^2$ the state vector takes the form

$$\psi(x) = (\varkappa r)^{-1}e^{-\varkappa r} - g\delta(x), \quad (92)$$

and the equation for determining the bound states

$$(g/2\pi)\varkappa^3 + \alpha_0\varkappa + 1 = 0 \quad (93)$$

has third degree and for $g=0$ goes over into the corresponding equation for the bound states of the model in Example 1.

Example 3. Quantum δ-functional potential acting in the p state.

This problem differs appreciably from Example 1, as can be seen from the point of view of the theory of extensions of symmetric operators. The spectral properties of the Laplacian on the space $L_2(R^3)$ are determined by the properties of the radial operator $\Delta_l = \partial_r^2 + 2/r\partial_r - l(l+1)/r^2$ on $L_2(R_+, r^2dr)$ $(R_+ = \{x\in R^1,\ x\geq 0\})$.

The operator Δ_l is unitarily equivalent to the operator $\Delta_l' = \partial_r^2 - l(l+1)/r^2$ on the space $L_2(R_+, dr)$. The corresponding transformation is given by the rule $\varphi \to r\varphi$. A specific property of the case $l\neq 0$ is that for $l\geq 1$ the operator Δ_l' is essentially self-adjoint on the set $C_0^\infty(R_+)$,[34] i.e., has a unique self-adjoint extension on $L_2(R_+, dr)$ equal to the operator Δ_l'. However, in such cases one can have nontrivial extensions in a space with indefinite metric, as was first noted in Ref. 35 for the example of the Lee model.

To obtain such extensions corresponding to a δ potential in the p state, it is necessary to modify the general scheme of construction of singular potentials. The first stage is to choose the original function space Ψ; for the given problem, this is done as follows. Let $\psi(x)$ be a function that is smooth for $x\neq 0$ and decreases rapidly at infinity. Its expansion with respect to spherical harmonics has the form

$$\psi(x) = \sum C_{lm}Y_{lm}(\mathbf{n})\, r^l\psi_l(r). \quad (94)$$

Further, it is assumed that the functions $\psi_l(r)$ for all $l\neq 1$ are even, infinitely differentiable functions of r, and that for $l=1$ the following representation holds in a neighborhood of the point $r=0$:

$$\psi_1(r) = \psi_s(r) + r^{-3}\psi_a(r), \quad (95)$$

where $\psi_s(r)$ and $\psi_a(r)=\varphi(r^2)$ are infinitely differentiable even functions in the neighborhood. The described set is chosen as the space Ψ. Let $\psi=\{C_{lm}, \psi_l\}$, $\chi=\{D_{lm}, \chi_l\}$ be a pair of functions in Ψ. In accordance with the rules for constructing the renormalized integral described in Sec. 2, there is defined on Ψ the sesquilinear form

$$(\chi,\psi) = \int d\mathbf{x}\chi^+(\mathbf{x})\psi(\mathbf{x}) = \sum_l\Big(\sum_m D_{lm}^*C_{lm}\Big)(4\pi)^{-1}\int d\mathbf{x}\chi_l^+(r)\psi_l(r)r^{2l}. \quad (96)$$

The integrals on the right-hand side are made three-dimensional to simplify integration by parts. The integral $I=\int d\mathbf{x}\, r^2\psi_1^+\psi_1$ is not positive definite. It is this that makes the metric indefinite.

The second stage in the solution of the original problem must consist of the restriction of the space Ψ to a new space with definite metric. In the given case, as we have already noted, this cannot be done. In the three stage, we first construct a Hamiltonian H that does not take us out of the space Ψ. Suppose $\psi\in\Psi$. Then in a neighborhood of the point $\mathbf{x}=0$

$$\Delta\psi = \sum_{l\neq 1}\sum_m C_{lm}\Delta[Y_{lm}(n)\, r^l\psi_l] + \sum_m C_{1m}\Delta[Y_{1m}(\mathbf{n})\, r\psi_s] + \sum_m C_{1m}\Delta[Y_{1m}(\mathbf{n})\, r^{-2}\psi_a]. \quad (97)$$

Only the last term in this equation contains terms that do not occur in ψ. The action of the Laplacian in the last term is given in accordance with the rules of the algebra in Sec. 2 by

$$\Delta(\mathbf{x}r^{-3}\psi_a) = \Delta(\mathbf{x}r^{-3}\varphi_a(r^2)) = \mathbf{x}r^{-3}[\Delta\varphi_a(r^2) - 8\varphi_a'] + 4\pi\nabla(\delta(\mathbf{x})\varphi_a).$$

It is now not difficult to write down a Hamiltonian that does not take us out of Ψ:

$$H\psi = -\Delta\psi + 4\pi C\nabla[\delta(\mathbf{x})\psi_a], \quad (98)$$

where $\mathrm{Cn} = \sum_m C_{1m}Y_{1m}(\mathbf{n})$.

Finally, the space Ψ must be restricted in accordance with the requirement $\mathrm{Im}(\psi, H\psi)=0$, which can be reduced by means of (98) to the form $\psi_s^*(0)\psi_a(0) = \psi_a^*(0)\psi_s(0)$. This last equation will be satisfied if we impose on the functions in Ψ the subsidiary condition

$$\psi_a(0) = -3\alpha\psi_s(0), \quad (99)$$

where α is an arbitrary real number. To each value of α there corresponds a set $\Psi_H\subset\Psi$ on which the operator H is symmetric.

Solving directly the Schrödinger equation with the boundary condition (99) for states with $l=1$ and $E=k^2$, we can obtain the radial eigenfunctions $\psi=\psi_{1k}(r)$:

$$\psi_{1k}(r) = (kr)^{-3/2}[\cos\delta_k J_{3/2}(kr) - \sin\delta_k J_{-3/2}(kr)], \quad (100)$$

where $J_\nu(\mathbf{x})$ is a Bessel function, and the p-wave scattering phase shift is related to the constant α by $\alpha k^3\cot\delta_k = -1$. The total cross section in this case is

$$\sigma = 4\pi k^2\alpha^2/(1+k^6\alpha^2). \quad (101)$$

For $\alpha<0$, there exists one bound state with energy $E=-\varkappa^2$, for which $\alpha\varkappa^3=-1$, and the radial eigenfunction $\psi_1(r)=\psi_{1\varkappa}(r)$ is expressed by

$$\psi_{1\varkappa}(r) = (\varkappa^{5/2}/\sqrt{3\pi})(\varkappa r)^{-3/2}K_{3/2}(\varkappa r), \quad (102)$$

where $K_{3/2}(\varkappa r)$ is a Macdonald function. For $\alpha>0$, it can be shown that the metric on the subspace generated by the complete set of eigenfunctions (100) is positive definite.[7] For $\alpha<0$, there is positivity of the metric for the continuum functions as well. However, for a bound state this is not the case. Direct calculation using the renormalization procedure gives $I=\int d\mathbf{x}\, r^2\psi^*_{1\varkappa}\psi_{1\varkappa}=-1$. Thus, the bound state has negative norm and is physically unacceptable. Therefore in the considered case the space Ψ_{H_2} must be restricted to the space Ψ_{H_3} generated by the vectors $\psi(x)+\psi_{1\varkappa}(\mathbf{x})$ $(\psi_{1\varkappa}, \psi)$ orthogonal to $\psi_{1\varkappa}$, which thereby have definite metric. Physically, this evidently means that for $l=1$ a bound state cannot exist in the scattering-length approximation. It is possible that bound states with positive norm will exist when allowance is made for the effective range, i.e., when more singular terms are added to the potential.

The following example generalizes Example 2 to the case of the inclusion of an external electromagnetic field and demonstrates the general method of Sec. 4 when the interaction depends on angular variables.

Example 4. Interaction of a charged particle with an external electromagnetic field in the presence of a strongly singular potential.

In what follows, the potentials $\mathbf{A}(\mathbf{x})$ and $A_0(\mathbf{x})$ of the electromagnetic field are assumed to be smooth functions of the coordinates with no explicit time dependence. We set $c=h=2m=1$. In the first stage, we choose a space Ψ consisting of elements of the form

$$\psi(\mathbf{x})=\psi_f(\mathbf{x})+\delta_A(\mathbf{x})\psi_1 \tag{103}$$

such that $\psi_f(\mathbf{x})$ are square-integrable functions, smooth everywhere apart from the origin; ψ_1 are complex numbers; and $\delta_A(\mathbf{x})=[1+ie\mathbf{x}\cdot\mathbf{A}(0)]\delta(\mathbf{x})$. In the neighborhood of the origin, the functions $\psi_f(\mathbf{x})$ admit the representation

$$\psi_f(\mathbf{x})=r^{-1}\psi_a(\mathbf{n})+\psi_s(\mathbf{n})+r\psi_r(\mathbf{x}). \tag{104}$$

where $\mathbf{n}=\mathbf{x}/r$; $\psi_a(\mathbf{n})$, $\psi_s(\mathbf{n})$, $\psi_r(\mathbf{n})$ are sufficiently smooth functions on the sphere and in R^3, respectively. The sesquilinear form on Ψ is defined like the form (84):

$$(\chi,\psi)=\int d\mathbf{x}\chi_f^*\psi_f+(\chi_f,\delta_A)\psi_1+\chi_1^*(\delta_A,\psi). \tag{105}$$

For its complete determination, it is sufficient to know $(\ldots)$ on the elements δ and ψ_f. By definition,

$$(\psi_f,\delta)=(4\pi)^{-1}\int d\Omega\psi_s(\mathbf{n})=[\psi_s(\mathbf{n})]_0.$$

Then the form (105) becomes

$$(\chi,\psi)=\int d\mathbf{x}\chi_f^*\psi_f+[\chi_A]_0^*\psi_1+\chi_1^*[\psi_A]_0, \tag{106}$$

where $\psi_A(\mathbf{n})=\psi_s(\mathbf{n})-ie\mathbf{n}\cdot\mathbf{A}(0)\psi_a(\mathbf{n})$. Such a form is not positive definite.

In the second stage, we make a transition to the space $\Psi_+\subset\Psi$ with positive-definite form

$$\Psi_+=\{\psi\in\Psi\mid\psi_1=g[\psi_A(\mathbf{n})]_0,\ g>0\}.$$

The form $(\ldots)$ defines on the space Ψ_f a scalar product, the completion with respect to it leading to the Hilbert space $\mathcal{H}$.

The third stage is the construction of the Hamiltonian for the posed problem. Let $D\subset\Psi_+$ be the set of elements for which

$$\psi_a(\mathbf{n})=\psi_a,\ \psi_s(\mathbf{n})=\psi_s+ie\mathbf{n}A(0)\psi_a.$$

In particular, for these elements $\psi_1=g\psi_s$. Suppose, in addition, $\Delta_A=(-i\nabla-e\mathbf{A}(x))^2$. A characteristic property of the region D is that if $\psi\in D$, then the representation (104) holds for the function $[\Delta_A\psi]_f$. On elements of D there is defined the operator H^A specified by

$$H^A\psi=\{[-\Delta_A+eA_0(\mathbf{x})]\}_f+g\delta_A(\mathbf{x})\times\{[-\Delta_A\psi+eA_0(\mathbf{x})\psi]_A\}_0. \tag{107}$$

The operator H^A is not symmetric on D. The necessary subset is distinguished by the condition $\mathrm{Im}(\psi, H\psi)=0$, which can be solved explicitly if we impose the boundary conditions

$$\psi_a=\alpha\psi_s-g(2\pi)^{-1}\{[\Delta_A\psi]_A\}_0,\ \alpha^*=\alpha. \tag{108}$$

These conditions define a dense subset in D, $D_\alpha\subset D$, on which the operator H^A is symmetric. The closure of H^A with domain of definition D_α in the space $\mathcal{H}$ gives the Hamiltonian of the system. It should be noted that the stationary Schrödinger equation $(H-E)\psi=0$ is invariant with respect to gauge transformations:

$$\left.\begin{aligned}&A_i\to A_i+\nabla_i\chi;\\&\psi\to\psi'=\psi\exp(ie\chi),\end{aligned}\right\} \tag{109}$$

where $\chi(\mathbf{x})$ is an arbitrary smooth function. Indeed, under such transformations

$$\psi_s\to\psi_s\exp[ie\chi(0)],\ \psi_a\to\psi_a\exp(ie\chi(0)),\quad\{[\Delta_A\psi]_A\}_0\to\{[\Delta_A\psi]_A\}_0\exp[ie\chi(0)],$$

from which one can readily see the invariance of the boundary conditions and the Schrödinger equation.

The constructed model makes it possible to find the corrections to the solutions for the model of Example 2 due to the electromagnetic field. For this, it is necessary to determine the Hamiltonian V of the interaction with the external field, since as yet only the total Hamiltonian H^A is defined on the space Ψ_+. Before we define the operator V, we must note the following circumstance. The operator H from Example 2 and the operator H^A must be referred to a common domain of definition. We subject the operator H with domain of definition Ψ_H to a unitary transformation, which we specify as the operator of multiplication by the function $\exp[ie\int_0^1 ds\,\mathbf{x}\cdot\mathbf{A}(\mathbf{x},s)]$, after which H goes over into a certain operator H^0. The domain of definition of the operator H^0 is specified like the domain of definition D_α of H^α with replacement of $A(x)$ by $\nabla[\int ds\,\mathbf{x}\cdot\mathbf{A}(\mathbf{x}s)]$. By means of the formula[36]

$$A(\mathbf{x})=\nabla\left[\int_0^1 ds\,\mathbf{x}A(\mathbf{x}s)\right]-\left[\mathbf{x},\int_0^1 s\,ds\mathbf{B}(\mathbf{x}s)\right], \tag{110}$$

where $\mathbf{B}=\mathrm{curl}\mathbf{A}$, it is easy to show that such a replacement does not change the dependence on A of the number $\{[\Delta_A\psi]_A\}_0$ in the boundary conditions. Thus, the domains of definition of H^0 and H^A coincide. The explicit form of H^0 is obtained by replacing in (107) the

potential $A(x)$ by $\nabla[\int ds\,\mathbf{x}\cdot\mathbf{A}(\mathbf{x}s)]$ and the potential $A_0(\mathbf{x})$ by $A_0(0)$. This last substitution amounts to reduction of the spectra of H^0 and H^A to a common origin. One can subject to this transformation the Hamiltonian H^A, without transforming the Hamiltonian without an external field. There is then a transition to a formulation of the problem without a potential, in which the interaction with the magnetic field is nonlocal. Such a formulation of electrodynamics was considered in Ref. 36. We can now define the Hamiltonian of the interaction with the external field as $V=H^A-H^0$ and use perturbation theory in physically justified cases. As an example, the first-order corrections to the energies of the bound states of a particle moving in the field of a strongly singular potential that are due to an external homogeneous magnetic field $A_0=0$, $\mathbf{A}=-1/2[\mathbf{x}\times\mathbf{B}]$ were found in Ref. 8. It is sufficient to consider the operator V only on spherically symmetric vectors. In this case $V=(e^2B^2/4)r^2\sin\theta$, $\mathbf{x}\cdot\mathbf{B}=rB\cos\theta$. The normalized solution of the equation $H^0\psi=-\varkappa^2\psi$ has the form

$$\psi_{\mathrm{bd}}=[\varkappa/2\,(\pi+g\varkappa^3)]^{1/2}\,[r^{-1}\exp(-\varkappa r)-g\varkappa\delta(\varkappa)],$$

where $\varkappa=\varkappa(\alpha, g)$ is determined by Eq. (93). The first correction to the level $-\varkappa^2$ is given by

$$E^{(1)}=\int d\mathbf{x}\psi_{\mathrm{bd}}^{+}V\psi_{\mathrm{bd}}=\frac{\pi e^2B^2}{12\varkappa^2(\pi+g\varkappa^3)}. \tag{111}$$

6. FREE-SOLUTION REPRESENTATION FOR SCHRÖDINGER EQUATIONS WITH STRONGLY SINGULAR POTENTIALS

A remarkable feature of the considered models corresponding to concentrated singular potentials is that one can construct for them a representation in which the initial Schrödinger equation reduces to a free equation. The transformation to such a representation is not specified by any kernel. However, its inverse does have a kernel and a simple form. This last circumstance makes it possible to obtain solutions of the original equations with singular potentials from the solutions for the free equations, and it may be helpful in a number of problems.

Let H be the Hamiltonian (85) with domain of definition Ψ_H^0 that characterizes the model from Example 2 in Sec. 5. In general, when the operator H is applied to vectors in Ψ_H^0 it carries them out of this space. Let $\Psi_{H_1}\subset\Psi_H^0$ be the subspace for which H does not do this: $H\psi\in\Psi_{H_1}$ if $\psi\in\Psi_{H_1}$. It follows from this that the condition (88) must be satisfied for the elements $H^n\psi$ for any positive integer n. To obtain the necessary conditions, it is convenient to introduce averaging over the angles:

$$\psi_0(\mathbf{x})=(4\pi)^{-1}\int d\Omega\psi_f(\mathbf{x}).$$

Then in a neighborhood of the origin we have the representation

$$\left.\begin{aligned}&\psi_0(\mathbf{x})=\psi_{s0}(\mathbf{x})+r^{-1}\psi_a(\mathbf{x});\\&\psi_{s0}(\mathbf{x})=\psi_{s0}(r),\quad \psi_a(\mathbf{x})=\psi_a(r),\end{aligned}\right\} \tag{112}$$

where $\psi_{s0}(r)$ and $\psi_a(r)$ are infinitely differentiable functions. Parametrizing the Hamiltonian H by the quantities g and α, we can rewrite the condition (88) in the form

$$[\psi_a(r)]_{r=0}=[\alpha\{r\psi_{s0}(r)\}'-(2\pi)^{-1}g\{r\psi_{s0}(r)\}'']_{r=0} \tag{113}$$

(the prime denotes differentiation with respect to r). Since the radial part of the Laplacian is $r^{-1}\partial_r r$, under the action of the Hamiltonian H the function ψ_a goes over into ψ_a'', and the function $\{r\psi_{s0}(r)\}$ into $\{r\psi_{s0}(r)\}''$. Hence, the complete system of conditions imposed on the functions of the space Ψ_{H_1} will have the form

$$[\psi_a^{(2n)}]_{r=0}=[\alpha\{r\psi_{s0}\}^{(2n+1)}-(2\pi)^{-1}g\{r\psi_{s0}(r)\}^{(2n+3)}]_{r=0},\quad n=0,1,2,\ldots \tag{114}$$

The coefficients $[\psi_a^{(2n)}(r)]_{r=0}$ and $[\{r\psi_{s0}\}^{(2n+1)}]_{r=0}$ can be expressed in terms of $\psi(\mathbf{x})$ by means of the renormalized integrals

$$[\{r\psi_{s0}\}^{(2n+1)}]_{r=0}=\int d\mathbf{x}\,\delta(\mathbf{x})\,r^{-1}(\mathbf{x}\nabla)\,r\Delta^n\psi;$$
$$[\psi_a^{(2n)}]_{r=0}=\int d\mathbf{x}\delta(\mathbf{x})\,r\Delta^n\psi.$$

The set Ψ_{H_1} contains the necessary integrals (and sums in the presence of bound states) over the eigenfunctions of the operator H and is thus dense in $\mathscr{H}$.

Now let $\Psi_{H_2}\subset\Psi_{H_1}$ be the subset of elements for which ψ_s and ψ_a are entire functions. Then we can sum the Taylor series with coefficients from the left- and right-hand sides of the relation (114), which leads to an explicit expression for $\psi_a(r)$ in terms of $\psi_{s0}(r)$ in the complete space:

$$\psi_a(r)=\alpha\{r\psi_{s0}(r)\}'-(2\pi)^{-1}g\{r\psi_{s0}(r)\}''. \tag{115}$$

For the functions $\psi_a(\mathbf{x})$ and $\psi_{s0}(\mathbf{x})$, the same expression can be rewritten in the form

$$\psi_a(\mathbf{x})=\alpha(1+\mathbf{x}\nabla)\psi_{s0}(\mathbf{x})-(2\pi)^{-1}g(1+\mathbf{x}\nabla)\Delta\psi_{s0}(\mathbf{x}). \tag{116}$$

By means of the relations (115), the functions $\psi(\mathbf{x})$ can be uniquely expressed in terms of $\psi_s(\mathbf{x})$. Indeed for waves with $l\neq0$ the equations $\psi_l(r)=\psi_{sl}(r)$ hold, and for waves with $l=0$ the required expression can be obtained by means of Eqs. (112) and (113). In Ψ_{H_2}, the inverse transformation is also possible. For waves with $l\neq0$, $\psi_{sl}=\psi_l(r)$. For waves with $l=0$, the coefficients $[\psi_{s0}^{(2n)}(r)]_{r=0}$ can first be expressed in terms of ψ by means of the renormalized integral (see Sec. 2):

$$[\psi_{s0}^{(2n)}]_{r=0}=\int d\mathbf{x}\,\delta(\mathbf{x})\,r\Delta^n(r^{-1}\psi). \tag{117}$$

After this, the function $\psi_{s0}(r)$ is obtained by summation of the Taylor series

$$\psi_{s0}(r)=\sum_{n=0}^{\infty}r^{2n}[\psi_{s0}^{(2n)}(r)]_{r=0}/(2n)! \tag{118}$$

The relations (117) and (118) solve the problem of constructing the function ψ_{s0}, given ψ, i.e., the problem of the transition from $\psi(\mathbf{x})$ to $\psi_s(\mathbf{x})$ for waves with $l=0$. Let Ψ_{Hs} be the set of functions $\psi_s(\mathbf{x})$. The scalar product (84) induces a scalar product in Ψ_{Hs}:

$$(\chi_s,\psi_s)=\int d\mathbf{x}\chi_f^*\psi_f+2g\chi_s^*(0)\,\psi_s(0), \tag{119}$$

where it is assumed that the functions χ_f and ψ_f are expressed in terms of χ_s and ψ_s. The formulation of the original problem expressed in the space Ψ_{Hs} will be

called the free-solution representation.

Property 1. The transition from Ψ_{H_2} to Ψ_{H_s} is made by means of a transformation that includes analytic continuation from some neighborhood of the origin to the complete space. In particular, to realize the transition it is sufficient to have the function ψ specified in a neighborhood of the point $\mathbf{x}=0$. But if the function is specified everywhere except in some neighborhood of the origin, an analytic continuation of ψ must also be made to realize the transition to ψ_s. It is thus clear that the transformation from Ψ_{H_2} to Ψ_{H_s} does not have a kernel.

Property 2. In the free-solution representation, the Hamiltonian H becomes free:

$$H\psi_s = -\Delta\psi_s. \tag{120}$$

This is already obvious from the infinite differentiability of the functions and can be readily established directly. The importance of Property 2 is emphasized by the name of the representation Ψ_{H_s}.

Property 3. If for the Hamiltonian H there exist bound states, then the functions $\psi_s(\mathbf{x})$ describing these states have exponential growth at infinity (the norm being finite). This property follows from the form of the solutions for a bound state and will be demonstrated below.

It follows from the existence of the transition from Ψ_{H_s} to Ψ_{H_2} and from Property 2 that the solution of the original Schrödinger equation

$$i\partial_t\psi = H\psi \tag{121}$$

with the Hamiltonian (86) describing a nontrivial strongly singular interaction reduces to the solution of the free equation. In accordance with Property 3, to obtain the complete solution we must ensure that the exponentially growing solutions corresponding to bound states are not omitted. The complete solution of Eq. (121) by the method of transition to the free-solution representation is obtained as follows. In accordance with Eqs. (114) and (120), each free solution $\exp\{-i\omega_k t + i\mathbf{k}\cdot\mathbf{x}\}$, $\omega_k = k^2$, will correspond to the solution $\exp(-i\omega_k t)\psi_k(\mathbf{x})$ of Eq. (121), where

$$\psi_k(\mathbf{x}) = \exp(i\mathbf{k}x) + r^{-1}[\alpha + (2\pi)^{-1}gk^2]\cos kr + g\delta(\mathbf{x}),\ k = |\mathbf{k}|. \tag{122}$$

The complete solution of Eq. (121) is

$$\psi(\mathbf{x}, t) = \int d\mathbf{k}\exp(-i\omega_k t)\psi_k(\mathbf{x})\,b(\mathbf{k}) + \sum b_j\psi_j(\mathbf{x})\exp(-iE_j t), \tag{123}$$

where $b(\mathbf{k})$ is an arbitrary function in a space whose form can be determined more precisely if necessary, b_j are complex numbers, $\psi_j(\mathbf{x})$ are bound-state functions, and j is the index that labels the bound states. We should note two properties of the general solution (123) which are important in that they are preserved in generalizations.

Property 4. From the form of the Hamiltonian (120) it is not yet possible to obtain complete information about the bound-state functions. One can only say that the bound-state functions correspond to free solutions ψ_{sj} of the form

$$\psi_{sj}(\mathbf{x}) = (\varkappa_j r)^{-1}\sinh(\varkappa_j r),\ E_j = -\varkappa_j^2. \tag{124}$$

To obtain the number of bound states and their energy values it is also necessary to use the requirement of finiteness of the norm generated by the form (119).

Property 5. For the complete solution of the Cauchy problem it is necessary to express $b(\mathbf{k})$ and b_j in terms of $\psi(\mathbf{x}, 0)$.

To obtain the phase shifts and bound-state energies, we go over to the momentum representation for $\psi_k(\mathbf{x})$ and separate the waves $\psi_{0k}(\mathbf{p})$ with $l=0$:

$$\psi_{0k}(\mathbf{p}) = (4\pi)^{-1}\int d\Omega_p\,(2\pi)^{-3}\int d\mathbf{x}\exp(-i\mathbf{p}\mathbf{x})\,\psi_k(\mathbf{x}).$$

The result of the calculations can be represented in the form

$$\psi_{0k}(\mathbf{p}) = \frac{i}{4\pi^2 k}\left[\frac{1-(2\pi)^{-1}ik(2\pi\alpha+gk^2)}{k^2-p^2+i0} - \frac{1-(2\pi)^{-1}ik(2\pi\alpha+gk^2)}{p^2-k^2+i0}\right], \tag{125}$$

which is convenient for obtaining the "in" and "out" limits:

$$\psi_k\begin{pmatrix}\text{in}\\ \text{out}\end{pmatrix}(p) = \lim_{t\to\mp\infty}\exp[-i(k^2-p^2)t]\,\psi_{0k}(p).$$

Each term in the curly brackets in (125) contributes to only one of the limits

$$\psi_k\begin{pmatrix}\text{in}\\ \text{out}\end{pmatrix}(p) = -(2\pi k)^{-1}\delta(p^2-k^2)[1\mp(2\pi)^{-1}ik(2\pi\alpha+gk^2)]. \tag{126}$$

It follows from this that the phase shift δ_k is determined by

$$\tan\delta_k = (2\pi)^{-1}k(2\pi\alpha + gk^2).$$

The right-hand sides in (125) and (126) do not contain poles corresponding to bound states. However, there must be poles in the S matrix $S(k) = (1+i\tan\delta_k)/(1-i\tan\delta_k)$. Therefore, the function $\psi_{k\text{out}}(p)$ must have zeros with respect to the variable $\varkappa$, where $k = i\varkappa$, at the points of the bound states. These zeros correspond to real bound states for real $\varkappa > 0$ and poles of S in the unphysical region in the remaining cases. The bound states are described by Eq. (93).

In the considered case, the transition to the free-solution representation not only gives the general solution (123) but also makes it possible to obtain solutions of the scattering and bound-state problems. It is easy to show that the same can be done for the one-dimensional singular and strongly singular potentials considered in Sec. 4. A minor difference is that the functions ψ_s and ψ_a are expressed by relations of the type (116) in terms of a new function that satisfies the free equation.

CONCLUSIONS

In creating Refs. 1–9, Shirokov had in mind the problem of constructing suitable algebras of generalized functions for use in quantum field theory. There have remained only a few notes devoted to this problem, which he apparently regarded as premature. The most closely related problems were the follow-

ing[3,5]: 1) construction of new one-dimensional and multidimensional algebras containing δ, r^k, $k=0, \pm 1, \pm 2, \ldots$, and also generalized functions of other types, for example, x^k and multidimensional analogs of the functional η (see Sec. 3); 2) the problem of classifying physically inequivalent models with δ-functional potentials and the connection between the method of associative algebras of generalized functions and the methods of the theory of extensions of symmetric operators; 3) the construction of N-particle models with two-body δ-functional potentials. These problems were the subjects of several investigations by students of Shirokov. Thus, in Refs. 37 and 38 Tolokonnikov constructed an associative–commutative algebra generated by elements of the type δ, x^k, $k=0, \pm 1, \pm 2, \ldots$, classified differential rings containing $\delta(x)$, r^k, $x \in R^n$, $n=1, 2, \ldots$, and for odd-dimensional R^n constructed algebras including these elements. An algebra containing the functionals δ and r^k in the case of arbitrary dimension $d=2, 3, \ldots$ is constructed in Ref. 39. In Ref. 40, a correct model is constructed with a semibounded Hamiltonian on a Hilbert space different from L_2 for a system of three particles with δ-functional potentials. Shirokov's method of Refs. 1–9 found further use in the case of singular noncentral interactions of spin-$\frac{1}{2}$ particles in Ref. 41.

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