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Schrödinger operator in an overfull set

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Abstract. – When a wave function is represented as a linear combination over an overfull set of elementary states, an ambiguity arises since such a representation is not unique. We introduce a variational principle which eliminates this ambiguity, and results in an expansion which provides "the best" representation to a given Schrödinger operator.

Operational simplicity of an expansion of a wave function over a basis in the Hilbert space is an undisputable advantage for many non-relativistic quantum-mechanical computations. However, in certain cases, there are several "natural" bases at one's disposal, and it is not easy to decide which is preferable. Hence, it sounds attractive to use several bases simultaneously, and to represent states as expansions over an *overfull set* obtained by a junction of their elements. Unfortunately, as is well known, such a representation is not unique, and lacks many convenient properties of full sets (*e.g.*, explicit formulae to compute coefficients of expansions). Because of this objection, overfull sets are used less frequently than they, perhaps, deserve.

Let us consider a dense set Ω of the wave functions $\varphi(x,k)$ (elementary states), where x is the spatial variable, and k is a label which enumerates the states of Ω. The parameter k can be discrete and/or continuous. We assume, for simplicity, that $\varphi(x,k)$ are bound states of some known potentials. The density of the set Ω means that any normalized wave function $\psi(x)$ can be approximated with a superposition of wave functions $\varphi(x,k)$. Consider a formal expansion of a wave function ψ over the set Ω:

$$\psi(x)=\sum_k a(k)\varphi(x,k), \tag{1}$$

where $\sum_k$ is a summation over all the labels k (integration over continuous and summation over discrete values). Expression (1) is formal, and its coefficients, $a(k)$, are not defined. The rules of computation of $a(k)$ are the central point in question.

In this letter, we develop a formal method which eliminates the ambiguity of the expansion (1). The main features of our approach are

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i) We put the question of the expansion over the set Ω in connection with the Schrödinger operator under consideration (an accurate formulation will be given below).

ii) We seek such an expansion of the form (1), for which the Schrödinger operator acts most similarly to an operator of multiplication with a function. In other words, we are going to find an expansion for which the algebra associated with the Schrödinger operator has the simplest explicit representation.

Below, we cast these intuitive features into the form of a variational problem. It turns out that a formal solution to this problem results in a unique choice of expansion (extremal expansion), with explicit rules of computations for its coefficients $a(k)$. We finish the letter with an example of computations.

Preliminary discussion. Denote as $H = -\Delta + U$ the Schrödinger operator with the potential U of interest. The action of H on the formal expansion (1) may be written as $H\psi(x) = \sum_k a(k)h(x,k)\varphi(x,k)$. The functions $h(x,k)$ are defined by the action of H on the elementary states $\varphi(x,k)$, *i.e.* $H\varphi(x,k) = h(x,k)\varphi(x,k)$. Denote as $h(x,k)\cdot$ the operator of multiplication with the function $h(x,k)$. Generally speaking, the action of powers of H on the function $\varphi(x,k)$ is not identical to the action of powers of the operator $h(x,k)\cdot$. Indeed, $H^2\varphi(x,k) = H(h(x,k)\varphi(x,k)) \neq h^2(x,k)\varphi(x,k)$. Thus, if we define the operators $h(\cdot)$ and $h^2(\cdot)$ as

$$h(\psi(x)) = \sum_k a(k)h(x,k)\varphi(x,k),$$
$$h^2(\psi(x)) = \sum_k a(k)h^2(x,k)\varphi(x,k),$$

then $H^2\psi \neq h^2(\psi)$. Consequently, the *commutator* $[H, h(\cdot)]$ is not equal to zero:

$$[H, h(\cdot)]\psi(x) = \sum_k \{H[h(x,k)\varphi(x,k)] - h^2(x,k)\varphi(x,k)\}a(k) \neq 0. \tag{2}$$

Remark i). We are led to the consideration of two algebras. The first one is the usual algebra, Alg_H, whose elements are formal linear combinations of the powers H^m. The elements of the second algebra, Alg_h, act as linear combinations of the operators $h^m(\cdot)$, where $h^m(\psi(x)) = \sum_k a(k)h^m(x,k)\varphi(x,k)$. Because of the inequality (2), algebras Alg_H and Alg_h are different. Notice that our definition of the algebra Alg_h is essentially based on the formal expansion (1). Loosely speaking, Alg_H and Alg_h differ by the commutator (2).

After this preliminary consideration, we are able to formulate the problem of an *extremal expansion*. An expansion of the form (1) will be called extremal, if it gives a minimum to a difference from zero of the commutator (2), where the minimum is understood in some suitable sense. Specifically, we define the extremal expansion as a solution to the following variational problem:

$$A[a] = \|[H, h(\cdot)]\psi\|^2 \to \min, \quad \psi(x) = \sum_k a(k)\varphi(x,k). \tag{3}$$

Here $\|\cdot\|$ is the L^2-norm. The coefficients of the extremal expansions will be labeled with an asterisk: $a^*(k)$.

Remark ii). Let us discuss the sense of the problem (3). If the operators H and $h(\cdot)$ commute, then Alg_H coincides with Alg_h. This case is especially simple. Indeed, then the action of the functions of the operator H is given by explicit integrals in the k-space. For example, the evolution operator $U_H(t) = \exp[itH]$ acts on the function ψ as follows:

$U_H(t)\psi = \sum_k \exp[ith(x,k)]a(k)\varphi(x,k)$. On the other hand, with an overfull set Ω, we have the freedom to choose the coefficients of the expansion (1). We use this freedom to obtain the maximal simplification of the algebra Alg_H or, in other words, to minimize the deviation of the operator H^2 from its "integral piece" $h^2(\cdot)$.

In a general situation, a formal solution to the variational problem (3) exists and is unique. This solution should give us the desired rules for computation of the coefficients $a^*(k)$. Now we will derive an explicit form of these rules.

Formal solution. We denote $q(x,k) = [H, h(x,k)\cdot]\varphi(x,k)$. The functional $A[a]$ in the problem (3) may be written as

$$A[a] = \sum_k \sum_{k'} a(k) Q(k,k') \overline{a(k')},$$

where the overbar denotes complex conjugation, and where $Q(k,k') = \overline{Q(k',k)}$ is the kernel of a symmetric integral operator in the k-space:

$$Q(k,k') = \int \mathrm{d}x \; q(x,k)\overline{q(x,k')}.$$

In the following, we assume the nondegeneracy of the quadratic functional A (3), which amounts to invertibility of the operator Q, and this requirement is met in a general case where none of the elementary states $\varphi(x,k)$ is an eigenfunction of H. Denote as $Q_{-1}(k,k')$ the kernel of the integral operator Q^{-1}. Solving the problem (3) with the help of the Lagrange multipliers, we obtain two formulae which give the direct and the inverse transforms for the extremal expansion:

$$a^*(k) = \int \mathrm{d}x \; \lambda(x) \sum_{k'} Q_{-1}(k,k')\overline{\varphi(x,k')},$$

$$\psi(x) = \int \mathrm{d}x' \; K_{-1}(x,x')\lambda(x').$$

Here $K_{-1}(x,x') = \overline{K_{-1}(x',x)}$ is the kernel of a symmetric integral operator K^{-1} in the x-space:

$$K_{-1}(x,x') = \sum_k \sum_{k'} \varphi(x,k) Q_{-1}(k,k') \overline{\varphi(x',k')}.$$

Denoting as $K(x,x')$ the kernel of the inverse operator K, one can write down explicit expressions of direct and inverse transforms for the extremal expansion (3):

$$\begin{cases} a^*(k) = \int \mathrm{d}x \int \mathrm{d}x' K(x,x')\psi(x') \sum_{k'} Q_{-1}(k,k')\overline{\varphi(x,k')}, \\ \psi(x) = \sum_k a^*(k)\varphi(x,k). \end{cases} \tag{4}$$

Expressions (4) determine the extremal expansion over an overfull set of elementary states, and are our main result. Their properties have much in common with those of conventional expansions over an orthogonal basis. For example, formulae (4) result in the following identity:

$$\sum_k \sum_{k'} a^*(k) Q(k,k') \overline{a^*(k')} = \int \mathrm{d}x \int \mathrm{d}x' \psi(x) K(x,x') \overline{\psi(x')},$$

which reminds us of the usual $\sum_k |a(k)|^2 = \int \mathrm{d}x |\psi(x)|^2$ of an expansion over a basis.

Diagonal approximation. One can further simplify the problem of inversion of the two integral operators, Q and K^{-1}, required for the extremal expansion (4), by the weakening of the requirement (3). Namely, instead of the functional A let us consider another functional, $A_{\mathrm{D}} = \sum_k |a(k)|^2 \| [H, h(x,k)\cdot]\varphi(x,k)\|^2$, in the variational problem (3). Using the functional A_{D} instead of A amounts to a replacement of the kernel $Q(k,k')$ with its diagonal piece $Q_{\mathrm{D}}(k,k') = Q(k)\delta(k-k')$, where $Q(k) = \int \mathrm{d}x |q(x,k)|^2$. Invertibility of Q requires here that the function $Q(k)$ be nowhere zero. Within this diagonal approximation, the kernel $K_{-1}(x,x')$ takes the form

$$K_{-1}(x,x') = \sum_k Q^{-1}(k)\varphi(x,k)\overline{\varphi(x',k)}, \tag{5}$$

while the extremal expansion (4) becomes

$$\begin{cases} a^*(k) = \displaystyle\int \mathrm{d}x \int \mathrm{d}x' K(x,x') Q^{-1}(k)\psi(x)\overline{\varphi(x',k)}, \\ \psi(x) = \displaystyle\sum_k a^*(k)\varphi(x,k)\,. \end{cases} \tag{6}$$

Here $K(x,x')$ is the kernel of the inverse to the operator K^{-1} in the diagonal approximation. Thus, the diagonal approximation to the extremal expansion amounts to invertion of the operator K^{-1} with the kernel of a rather simple form (5).

Example. We will give a simple example of a situation when the set Ω contains both bound and free states. Let Ω be obtained by adding a single normalized function $\varphi_0(x)$ to the basis of plane waves $\varphi(x,\kappa) = \exp[i\kappa\cdot x]$. As above, let φ_0 be a bound state of a known potential U_0, *i.e.* $(-\Delta + U_0)\varphi_0 = E_0\varphi_0$. Considering the expansions of the form

$$\psi(x) = a_0\varphi_0(x) + \int \mathrm{d}\kappa\ a(\kappa)\varphi(x,\kappa), \tag{7}$$

and a given Schrödinger operator $H = -\Delta + U$, let us find out the value of the coefficient a_0^* in the corresponding extremal expansion. The variational principle (3) amounts to a minimization of the quadratic form

$$Q(0,0)|a_0|^2 + a_0\int \mathrm{d}\kappa\ Q(0,\kappa)\overline{a(\kappa)} + \overline{a_0}\int \mathrm{d}\kappa\ Q(\kappa,0)a(\kappa) + \int \mathrm{d}\kappa \int \mathrm{d}\kappa'\ a(\kappa)Q(\kappa,\kappa')\overline{a(\kappa')}, \tag{8}$$

subject to the constraint (7). The various coefficients in eq. (8) are

$$\begin{aligned} Q(0,0) &= \int \mathrm{d}x |q(x,0)|^2, \\ Q(0,\kappa) &= \int \mathrm{d}x q(x,0)\overline{q(x,\kappa)}, \\ Q(\kappa,0) &= \overline{Q(0,\kappa)}, \\ Q(\kappa,\kappa') &= \int \mathrm{d}x q(x,\kappa)\overline{q(x,\kappa')}, \end{aligned}$$

where the integrands are constructed with the help of the following functions:

$$\begin{aligned} q(x,0) &= \varphi_0\Delta(U_0 - U) + 2\nabla\varphi_0\cdot\nabla(U_0 - U), \\ q(x,\kappa) &= -\exp[i\kappa\cdot x][\Delta U + 2i\kappa\cdot\nabla U]. \end{aligned}$$

Now we find the minimum of the quadratic-in-a_0 expression (8), and using the constraint (7), derive the coefficient of the extremal expansion a_0^*:

$$a_0^* = -\frac{\int \mathrm{d}\kappa\ b(\kappa)Q(\kappa,0)}{Q(0,0) - \int \mathrm{d}\kappa\ b_0(\kappa)Q(\kappa,0)}. \tag{9}$$

Here $b(\kappa)$ and $b_0(\kappa)$ are conventional Fourier coefficients of the functions ψ and φ_0. Thus, eq. (9) gives a "share" of the bound state φ_0 in the "net" state ψ for the potential U. The example considered is easily extended to an arbitrary finite number of bound states, and the construction of the extremal expansion amounts to finding a minimum of a finite-dimensional quadratic form. We will close this letter with a number of comments.

i) We have demonstrated that the overfull sets can be operated largely in the same spirit as conventional full sets of elementary states. The key point is the variational principle (3), or its weaker version (the diagonal approximation). Otherwise stated, this is the request to simplify the representation of the algebra of a given Schrödinger operator. With this, we have done the first (and necessarily formal) step into the program of constructing an analog of operational calculus with the overfull sets.

ii) One of the advantages brought about by the extremal expansion is the trace formulae of operator-valued functions $\Phi(H)$. In the diagonal approximation, in particular, we are able to write for the trace $\mathrm{Tr}\Phi(H)$ an explicit integral representation: $\mathrm{Tr}\Phi(H) \sim \int \mathrm{d}x \Phi_H(x,x)$, where

$$\Phi_H(x,x') = \sum_k \int \mathrm{d}x'' Q^{-1}(k)K(x',x'')\Phi[h(x,k)]\varphi(x,k)\overline{\varphi(x'',k)}.$$

Here the "$\sim$" means that for the extremal expansion, the algebra of the operator H is most close to the algebra of its symbol [1], [2]. Techniques of inversion of the operators Q and K^{-1} can be borrowed from the so-called parametric expansions [1]-[3].

iii) A natural field of application of the suggested formalism seems to be studies of bound states in complex potentials, where the approach makes it possible to use several bases of solvable problems simultaneously. A description of neutral K-mesons might serve as an example. There, the overfull set appears as the junction of the states of K^0 and $\overline{\mathrm{K}}^0$ mesons with the decay states. It can be demonstrated [4] that the minimum principle (3) reduces to the minimum of the norm of the commutator of the weak and strong interaction Hamiltonians, and to compute the effective amplitudes of the K^0 and $\overline{\mathrm{K}}^0$ states. Details of the analysis will be reported separately [4].

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