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An algebraic approach to the inverse eigenvalue problem for a quantum system with a dynamical group

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Abstract. An algebraic approach to the inverse eigenvalue problem for a quantum system with a dynamical group is formulated for the first time. The one-dimensional problem is treated explicitly in detail for both the finite-dimensional and infinite-dimensional Hilbert spaces. For the finite-dimensional Hilbert space, the $su(2)$ algebraic representation is used; while for the infinite-dimensional Hilbert space, the Heisenberg–Weyl algebraic representation is employed. The Fourier expansion technique is generalized to the operator space, which is suitable for analysis of irregular spectra. The polynomial operator basis is also used for the complement, which is appropriate for analysis of some simple Hamiltonians. The proposed new approach is applied to solve the classical inverse Sturm–Liouville problem and to study the problems of quantum regular and irregular spectra.

1. Introduction

Quantum theory has two major problems for solution: the bound-state eigenvalue problem and the scattering or reaction problem. The direct problem of quantum mechanics is: given a Hamiltonian of a quantum system, compute all the data of the eigenvalue problem and the scattering or reaction problem. The inverse of the above problem is as follows: given a set of necessary and sufficient data, construct a Hamiltonian to reproduce this data. This is called the inverse problem of quantum theory.

In recent decades, a new physical–mathematical discipline—the theory of the inverse problem—has been developed rapidly. This nonlinear physical–mathematical theory has been a great achievement [1]: it has become an interdisciplinary study [2]. The quantum inverse theory addresses two major topics: the inverse scattering problem and the inverse eigenvalue problem. The former topic has received much more attention, and a large number of papers have been published in this field [1]. However, the latter topic has received relatively less attention.

Since the pioneering work of Borg [3] and Levinson [4] on the inverse Sturm–Liouville problem, the conventional inverse eigenvalue problem has addressed the recovery of the potential from knowledge of eigenenergies and eigenfunctions assuming that the kinetic energy operator of the Hamiltonian is given. Borg and Levinson stressed the need for two spectra for the recovery of the potential [3, 4]. Following the work of Krein [5] and Gel'fand and Levitan [6], it has become clear that one spectrum together with knowledge of the eigenfunctions at one end-point is sufficient to recover the potential.

Owing to the extensive and intensive study of nuclear physics and atomic physics, it is known that dynamical symmetry plays an important role in the microscopic world [7]. For instance, for many microscopic systems, such as the hydrogen atom, the diatomic molecule with Morse potential, the nuclear shell model and the nuclear collective model, their Hamiltonians can be expressed in terms of generators of a certain kind of dynamical group. This fact confirms Dirac's profound idea that quantum mechanics can be expressed in terms of some dynamical algebras [8]. For a system with a dynamical group, the important thing is not the division between the kinetic energy and the potential, it is the algebraic structure of the total Hamiltonian. Therefore, for a dynamical algebraic system, one still needs the method for solving the inverse problem. It is the purpose of this work to deal with the inverse eigenvalue problem for a quantum system with a dynamical group.

The need to address the quantum inverse eigenvalue problem has recently become urgent, because of the study of quantum chaos [9–11]. One major topic of quantum chaos is the statistical behaviour of the eigenstates of a quantum system. Many examples investigated have shown regular or chaotic behaviour of the energy spectra. But little information has been gained as to what the relation between the statistical property of the energy spectrum and the structure of the corresponding Hamiltonian is. To study the problem in general, one needs to establish the physical–mathematical connection between a Hamiltonian and its bound state data. The inverse eigenvalue theory addresses this problem and is very desirable. It is also the purpose of this work to deal with the inverse eigenvalue problem and its application to the spectrum problem of quantum chaos.

The paper is organized as follows. In section 2 we shall formulate the inverse eigenvalue problem for a system with a dynamical group in detail. We try to solve the problem not only in principle, but also in practice, i.e. to make it calculable. Some modern mathematical techniques are employed to make the problem solvable within the capacity of currently available computers. After the problem is properly posed in section 2.1, a general procedure for solution is sketched in section 2.2. The inverse problem for one dimension in configuration space and finite dimensions in Hilbert space is formulated in the representation of the nonlinear $su(2)$ algebra in section 2.3. Section 2.4 is devoted to the one-dimensional problem for infinite-dimensional Hilbert space in the representation of the nonlinear Heisenberg–Weyl algebra. In this section, the Fourier series expansion technique is generalized to the operator space. It is found that the Fourier series expansion technique in nonlinear operator space is a very powerful and elegant means of solving the problem. In section 2.5, the polynomial representation is given. It is found that the operator power basis and the polynomial basis are suitable for handling relatively simple Hamiltonians. For the highly nonlinear operator problems, they often yield violently fluctuating expansion coefficients. In contrast, the Fourier expansion technique in operator space is suitable for handling more complicated Hamiltonians, especially chaotic systems, just as it does in function space for the spectrum analysis of the noise of various waves. In section 3, the method developed above is applied to study first the classical inverse Sturm–Liouville problem, then the quantum regular spectra, and finally the problem of the quantum chaotic spectrum. The outlook and a discussion are given in section 4.

2. Quantum inverse eigenvalue problem

2.1. Specification of the problem

Before starting the main text, we should properly describe our problem to be solved in order to avoid misunderstanding. The inverse eigenvalue problem of quantum mechanics can be described by the following three categories:

(i) *Inverse problem within Heisenberg mechanics.* This is the matrix form of quantum mechanics. Here any operator including \hat{H} is a matrix. If E_n and ψ_n are given, the required Hamiltonian is just

$$\hat{H} = \sum_n E_n |\psi_n\rangle \langle \psi_n|. \quad (2.1)$$

However, this kind of solution is of little use, since \hat{H} is directly expressed in terms of the input data. It is too empirical to exploit its algebraic structure.

(ii) *Inverse problem within Dirac mechanics.* This is the algebraic form of quantum mechanics where any operator is a function of certain algebra $a = \{\hat{X}_\alpha\}$. For the Hamiltonian,

$$\hat{H} = H(\hat{X}_\alpha). \quad (2.2)$$

In this case, the inverse problem is not trivial. It is a complicated task to construct a Hamiltonian which is a nonlinear function of the algebraic generators \hat{X}_α and reproduces the given data. This is an intrinsic expression of \hat{H} since it is no longer expressed directly in terms of the empirical data, but expressed in terms of a certain algebra which dictates a Hilbert space. With the help of the algebra one could study the symmetry of the Hamiltonian. By virtue of the coherent state method, one can study the semiclassical and classical limit of the system.

(iii) *Inverse problem within Schrödinger mechanics.* This is the differential form of quantum mechanics where \hat{H} is expressed in terms of differential operators, for instance coordinates \hat{x} and momenta \hat{p} :

$$\hat{H} = H(\hat{x}, \hat{p}). \quad (2.3)$$

Since \hat{x} and \hat{p} constitute Heisenberg algebra, the inverse problem in fact belongs to category (ii) with the requirement that the algebra should take the differential form.

In this paper, we shall specify our inverse eigenvalue problem as category (ii) or (iii).

2.2. Procedure of solution

Now we restate our inverse eigenvalue problem as follows: given a set of eigenenergies E_n and eigenstates ψ_n in some representation space of a certain algebra, how can a Hamiltonian which is expressed in terms of the algebra and can reproduce the data E_n and ψ_n be constructed?

The problem will be solved in three steps:

(i) Construct a Hamiltonian \hat{H}_0 from a complete set of commuting operators (Cartan subalgebra for a Lie algebra for instance) of the algebra $\{\hat{h}_i\}$,

$$\hat{H}_0 = H_0(\hat{h}_i) \quad (2.4)$$

which should reproduce the eigenenergies. Suppose the eigensolutions of $\{\hat{h}_i\}$ are $|n\rangle$, namely

$$\hat{h}_i |n\rangle = n_i |n\rangle. \quad (2.5)$$

That \hat{H}_0 reproduces E_n means

$$\hat{H}_0|n\rangle = E_n|n\rangle \quad (2.6)$$

where

$$E_n = H_0(n_i). \quad (2.7)$$

The above equation determines \hat{H}_0 uniquely.

(ii) Construct a unitary operator \hat{U} in terms of $\{\hat{X}_\alpha\}$,

$$\hat{U} = U(\hat{X}_\alpha) \quad \hat{U}^\dagger = \hat{U}^{-1}. \quad (2.8)$$

which transforms $|n\rangle$ to $|\psi_n\rangle$, namely

$$|\psi_n\rangle = \hat{U}|n\rangle = \sum_m U_{nm}|m\rangle \quad (2.9)$$

where

$$U_{mn} = \langle n|\hat{U}|m\rangle. \quad (2.10)$$

The above equation uniquely determines \hat{U} .

(iii) The required Hamiltonian \hat{H} is

$$\hat{H} = \hat{U}\hat{H}_0\hat{U}^{-1} \quad (2.11)$$

since

$$\hat{H}|\psi_n\rangle = \hat{U}\hat{H}_0\hat{U}^{-1}|\psi_n\rangle = \hat{U}\hat{H}_0|n\rangle = E_n|\psi_n\rangle. \quad (2.12)$$

Thus the inverse problem becomes finding the operators \hat{H}_0 and \hat{U} . In the following we proceed to solve the problem explicitly for the one-dimensional case.

2.3. One dimension. Finite-dimensional Hilbert space

Since the $SU(2)$ group has only one kind of elementary excitation, i.e. (\hat{J}_+, \hat{J}_-) , it is a one-dimensional dynamical group and its irreducible representation spans a finite-dimensional Hilbert space. Therefore our discussion in this subsection is based on the $su(2)$ algebra: $su(2) = \{\hat{J}_+, \hat{J}_-, \hat{J}_z\}$. Assume an $su(2)$ IRR basis is $|jm\rangle$, such that

$$\hat{J}_z|jm\rangle = m|jm\rangle \quad m = -j, \dots, +j. \quad (2.13)$$

The Hilbert space is of $2j+1$ dimensions. Since we are working in a single j -representation, we shall drop the j -label when no confusion would be caused. Assume a set of data E_n and ψ_n is given in such a Hilbert subspace. The ψ_n can be expanded in terms of the $su(2)$ IRR basis,

$$|\psi_n\rangle = \sum_m U_{nm}|m\rangle. \quad (2.14)$$

Therefore, giving ψ_n and giving U_{nm} are equivalent. The inverse problem will be solved as follows:

(i) \hat{H}_0 . Since \hat{H}_0 is a function of the Cartan operator \hat{J}_z of $\mathfrak{su}(2)$, it can be expressed in terms of the Fourier series of \hat{J}_z in general,

$$\hat{H}_0 = \sum_p h_p \exp(i\alpha_p \hat{J}_z) \tag{2.15}$$

where $\alpha_p = 2\pi p / (2j + 1)$ ($p = -j, \dots, +j$), and h_p is to be determined. From equation (2.13), we have

$$\hat{H}_0 |m\rangle = E_m |m\rangle \tag{2.16}$$

where

$$E_m = \sum_p h_p \exp(i\alpha_p m). \tag{2.17}$$

The solution of h_p is

$$h_p = \frac{1}{2j + 1} \sum_m E_m \exp(-i\alpha_p m). \tag{2.18}$$

Since for any given E_n the solution (2.18) always exists and $h_{-p}^* = h_p$, the expansion (2.15) is justified and the Hermiticity of \hat{H}_0 is guaranteed.

(ii) \hat{U} . Next we shall find the operator \hat{U} which transforms the vectors $|m\rangle$ back to the given vectors ψ_m . Let the operator be expressed in terms of the products of two different rotations. Since there are $(2j + 1)^2$ components of \hat{U} in the Hilbert space, we express \hat{U} as

$$\hat{U} = \sum_{pq} D_{pq} \exp(i\alpha_p \hat{J}_\theta) \exp(i\alpha_q \hat{J}_y) \tag{2.19}$$

where \hat{J}_θ ($\theta = 0 - \pi$) is a rotation generator around some fixed axis and p, q are in the range $(-j, +j)$. This axis must be chosen to prevent the singularity of the solution in equation (2.19). The unitarity of \hat{U} will impose a restriction on D_{pq} . For simplicity we shall restrict this axis in the xy plane, making an angle of θ with the y -axis, namely

$$\hat{J}_\theta = \exp(-i\theta \hat{J}_z) \hat{J}_y \exp(i\theta \hat{J}_z). \tag{2.20}$$

Let us calculate

$$\begin{aligned} U_{mn} &= \langle n | \hat{U} | m \rangle \\ &= \sum_{p,q} D_{pq} \langle n | \exp(i\alpha_p \hat{J}_\theta) \exp(i\alpha_q \hat{J}_y) | m \rangle \\ &= \sum_{p,q} D_{pq} \langle n | \exp(-i\theta \hat{J}_z) \exp(i\alpha_p \hat{J}_y) \exp(i\theta \hat{J}_z) \exp(i\alpha_q \hat{J}_y) | m \rangle \\ &= \sum_{p,q} \sum_k \exp[i(k - n)\theta] d_{nk}^{(j)}(\alpha_p) d_{km}^{(j)}(\alpha_q) D_{pq}. \end{aligned} \tag{2.21}$$

The $d_{nm}^{(j)}(\alpha)$ are the usual d -functions as defined in [13]. We can express $d_{nm}^{(j)}(\alpha)$ as a sum of Fourier components,

$$d_{nm}^{(j)}(\alpha) = i^{n-m} \sum_k \Delta_{kn} \Delta_{km} \exp(-ik\alpha) \tag{2.22}$$

where

$$\Delta_{nm} \equiv d_{nm}^{(j)}\left(\frac{\pi}{2}\right). \quad (2.23)$$

Expand the d -functions in equation (2.21) with equation (2.22) and simplify it as follows:

$$\begin{aligned} U_{mn} &= \sum_{p,q} D_{pq} \sum_k \exp(-in\theta) \exp(ik\theta) i^{n-k} \sum_{k_1} \Delta_{k_1 n} \Delta_{k_1 k} i^{k-m} \\ &\quad \times \sum_{k_2} \Delta_{k_2 k} \Delta_{k_2 m} \exp(-ik_1 \alpha_p) \exp(-ik_2 \alpha_q) \\ &= \sum_{p,q} D_{pq} \sum_{k_1, k_2} \exp(-in\theta) i^{n-m; k_1-k_2} d_{k_1 k_2}^{(j)}(\theta) \Delta_{k_1 n} \Delta_{k_2 m} \\ &\quad \times \exp(-ik_1 \alpha_p) \exp(-ik_2 \alpha_q). \end{aligned} \quad (2.24)$$

Furthermore, since Δ_{mn} is real,

$$\begin{aligned} \sum_k \Delta_{k_1 k} \Delta_{k_2 k} &= \sum_k \Delta_{k_1 k} \Delta_{k_2 k}^* \\ &= \sum_k \langle k_1 | \exp\left(i\frac{\pi}{2} \hat{J}_y\right) | k \rangle \langle k | \exp\left(-i\frac{\pi}{2} \hat{J}_y\right) | k_2 \rangle \\ &= \delta_{k_1, k_2}. \end{aligned} \quad (2.25)$$

Equation (2.24) can be transformed as

$$\sum_{p,q} D_{pq} \exp(-ik_1 \alpha_p) \exp(-ik_2 \alpha_q) = \frac{i^{k_1-k_2}}{d_{k_1 k_2}^{(j)}(\theta)} \sum_{nm} \exp(in\theta) i^{m-n} \Delta_{k_1 n} \Delta_{k_2 m} U_{mn} \quad (2.26)$$

and the Fourier transformation gives the solutions of the coefficients D_{pq} ,

$$D_{pq} = \frac{1}{(2j+1)^2} \sum_{k_1, k_2} \left(\frac{i^{k_1-k_2}}{d_{k_1 k_2}^{(j)}(\theta)} \sum_{nm} \exp(in\theta) i^{m-n} \Delta_{k_1 n} \Delta_{k_2 m} U_{mn} \right) \exp(ik_1 \alpha_p) \exp(ik_2 \alpha_q). \quad (2.27)$$

The value of θ must be chosen carefully, so that none of the $d_{k_1 k_2}^{(j)}(\theta)$ vanish. In particular, we want to caution that, if θ is set to $\pi/2$, which corresponds to setting $\hat{J}_\theta = \hat{J}_z$, then the values of $d_{k_0}^{(j)}(\theta)$ and $d_{0k}^{(j)}(\theta)$ become zero for odd k in the even j case, and also for even k in the odd j case. However, the singularity does not occur for the case of half-integer j .

Finally, the Hamiltonian \hat{H} is related to \hat{H}_0 by a similar transformation:

$$\hat{H} = \hat{U} \hat{H}_0 \hat{U}^{-1}. \quad (2.28)$$

2.4. One dimension. Infinite-dimensional Hilbert space

Since the irreducible representation of the one-dimensional Heisenberg–Weyl (HW) group spans an infinite-dimensional Hilbert space, we are now working in the HW algebraic representation. For the coordinate \hat{x} and momentum \hat{p} , the HW algebra is

$$hw = \{\hat{x}, \hat{p}, \hat{n} = \frac{1}{2}(\hat{p}^2 + \hat{x}^2 - 1)\}. \tag{2.29}$$

Its generators satisfy the following commutator relations:

$$[\hat{x}, \hat{p}] = i \quad [\hat{n}, \hat{x}] = -i\hat{p} \quad [\hat{n}, \hat{p}] = i\hat{x}. \tag{2.30}$$

The IRR basis $|n\rangle$ is the eigenfunction of \hat{n} ,

$$\hat{n}|n\rangle = n|n\rangle \tag{2.31}$$

which is just the eigenfunction of one-dimensional harmonic oscillator.

(i) \hat{H}_0 . Since \hat{H}_0 is a function of the Cartan operator \hat{n} , it can be expressed in terms of the following Fourier series:

$$\hat{H}_0 = \lim_{N \rightarrow \infty} \sum_{p=1}^N [h_p \exp(i\alpha_p \hat{n}) + h_p^* \exp(-i\alpha_p \hat{n})] \tag{2.32}$$

where $\alpha_p = 2\pi p/(N + 1)$ and $N + 1$ represents the dimension of the Hilbert space. It should be remarked that the limit $N \rightarrow \infty$ in equation (2.32) is in a weak sense which is suitable for a practical calculation (the same is true for equations (2.51) and (2.52)). In fact, for a practical calculation, one can only work in a truncated subspace with a finite dimension, and N thus becomes a large integer. From equations (2.31) and (2.32), we have

$$\hat{H}_0|m\rangle = E_m|m\rangle \tag{2.33}$$

where

$$E_m = \lim_{N \rightarrow \infty} \sum_{p=1}^N [h_p \exp(i\alpha_p m) + h_p^* \exp(-i\alpha_p m)]. \tag{2.34}$$

The solution of h_p is

$$h_p = h_{N+1-p}^* = \lim_{N \rightarrow \infty} \frac{1}{2(N + 1)} \sum_{m=0}^N E_m \exp(-i\alpha_p m). \tag{2.35}$$

Since for any given E_m the solution (2.35) always exists, the expansion (2.32) is thus justified and the Hermiticity of \hat{H}_0 guaranteed.

(ii) \hat{U} . Assume

$$\hat{U} = \int dr ds D_{rs} \exp(ir\hat{x}) \exp(is\hat{p}). \tag{2.36}$$

The unitarity of \hat{U} imposes a restriction on D_{rs} . Let us calculate

$$U_{mn} = \langle n|\hat{U}|m\rangle = \int dr ds D_{rs} \langle n|\exp(ir\hat{x}) \exp(is\hat{p})|m\rangle. \tag{2.37}$$

Introducing the plane wavefunction,

$$|\psi_k(x)\rangle = \frac{1}{\sqrt{2\pi}} \exp(ikx) \quad (2.38)$$

and multiplying $\langle m|\exp(-is\hat{p})\exp(-ir\hat{x})|n\rangle$ from both sides of equation (2.37) and summing over m and n , we obtain

$$\begin{aligned} \text{LHS} &= \sum_{mn} U_{mn} \langle m|\exp(-is\hat{p})\exp(-ir\hat{x})|n\rangle \\ &= \sum_{mn} U_{mn} \int dk \langle m|\psi_k\rangle \langle \psi_{k+r}|n\rangle \exp(-isk) \end{aligned} \quad (2.39)$$

and

$$\begin{aligned} \text{RHS} &= \int dr' ds' D_{r's'} \text{Tr}\{\exp[-i(r-r')\hat{x}]\exp[-i(s-s')\hat{p}]\} \\ &= 2\pi D_{rs}. \end{aligned} \quad (2.40)$$

Therefore, the solution is

$$D_{rs} = \frac{1}{2\pi} \sum_{mn} U_{mn} \int dk \langle m|\psi_k\rangle \langle \psi_{k+r}|n\rangle \exp(-isk). \quad (2.41)$$

Further manipulation [14] yields

$$\begin{aligned} D_{rs} &= \frac{1}{2\pi} \exp\left(ir s - \frac{s^2 + r^2}{4}\right) \\ &\quad \times \left\{ \sum_{n \geq m} U_{mn} \sqrt{\frac{2^n m!}{2^m n!}} \left(-\frac{s+ir}{2}\right)^{n-m} L_m^{n-m}\left(\frac{s^2+r^2}{2}\right) (2 - \delta_{nm}) \right\} \end{aligned} \quad (2.42)$$

where L_m^n is a Laguerre function.

2.5. Polynomial representation

As was pointed out in the introduction, the above Fourier expansion technique is suitable for treating a complicated Hamiltonian. For a simple Hamiltonian, it is more convenient to employ a polynomial representation. To solve the problem, we write the Hamiltonian as

$$\hat{H} = \hat{H}_0 + \hat{V} \quad (2.43)$$

where \hat{H}_0 and \hat{V} are to be determined from the diagonal and off-diagonal matrix elements of \hat{H} , respectively, and H_{mn} are given in a basis diagonalizing \hat{H}_0 .

2.5.1. *Finite-dimensional Hilbert space. su(2) representation.* In such a case, we write \hat{H}_0 and \hat{V} as

$$\hat{H}_0 = \sum_{p=0}^{2j} h_p T_p(\hat{J}_z/j) \tag{2.44}$$

and

$$\hat{V} = \sum_{p,q=1}^{2j} D_{p,q} [T_p(\hat{J}_z/j) \hat{J}_+^q + \hat{J}_-^q T_p(\hat{J}_z/j)]. \tag{2.45}$$

Where T_p is the Chebyshev polynomial of the first kind. The diagonal elements of \hat{H} determine the structure of \hat{H}_0 ,

$$H_{mm} = \langle m | \hat{H} | m \rangle = \sum_{p=0}^{2j} h_p T_p(m/j). \tag{2.46}$$

The h_p can be obtained from the above equation. As j is very large, one has

$$h_p = \frac{2 - \delta_{p0}}{(2j + 1)\pi} \sum_m H_{mm} T_p\left(\frac{m}{j + \frac{1}{2}}\right) \left[1 - \left(\frac{m}{j + \frac{1}{2}}\right)^2\right]^{-1/2}. \tag{2.47}$$

The off-diagonal elements of \hat{H} can be used to determine \hat{V} , namely

$$H_{mn} = \sum_{p,q=1}^{2j} D_{pq} [T_p(m/j) V_{mn}^{q+} + V_{mn}^{q-} T_p(n/j)] \tag{2.48}$$

from which the coefficients D_{pq} can be obtained. Here,

$$V_{mn}^{q+} = \langle m | \hat{J}_+^q | n \rangle \quad V_{mn}^{q-} = \langle m | \hat{J}_-^q | n \rangle. \tag{2.49}$$

2.5.2. *Infinite-dimensional Hilbert space. HW representation.* In this case, we assume

$$\hat{H}_0 = \lim_{N \rightarrow \infty} \sum_{p=0}^N h_p T_p[(2\hat{n} - N)/N] \tag{2.50}$$

and

$$\hat{V} = \lim_{N \rightarrow \infty} \sum_{p,q=1}^N D_{pq} \{T_p[(2\hat{n} - N)/N] (\hat{x} - i\hat{p})^q + (\hat{x} + i\hat{p})^q T_p[(2\hat{n} - N)/N]\}. \tag{2.51}$$

The diagonal elements of \hat{H} are used to determine the \hat{H}_0 ,

$$H_{mm} = \lim_{N \rightarrow \infty} \sum_{p=0}^N h_p T_p[(2m - N)/N] \tag{2.52}$$

which yields the solution

$$h_p = \lim_{N \rightarrow \infty} \frac{2 - \delta_{p0}}{(N+1)\pi} \sum_{n=0}^N H_{nn} T_p \left(\frac{2n-N}{N+1} \right) \left[1 - \left(\frac{2n-N}{N+1} \right)^2 \right]^{-1/2}. \quad (2.53)$$

The \hat{V} or D_{pq} are determined by the off-diagonal elements of \hat{H} ,

$$H_{mn} = \lim_{N \rightarrow \infty} \sum_{p,q=1}^N D_{pq} \{ T_p [(2m-N)/N] X_{mn}^q + X_{nm}^{q*} T_p [(2n-N)/N] \} \quad (2.54)$$

where

$$X_{mn}^q = \langle m | (\hat{x} - i\hat{p})^q | n \rangle \quad (2.55)$$

and $|m\rangle$ is the eigenfunction of \hat{n} .

It should be pointed out that the matrix elements of \hat{H} , H_{mn} , can be calculated from the input data E_n and ψ_n .

3. Application

3.1. One-dimensional inverse Sturm–Liouville problem

The inverse Sturm–Liouville problem is usually formulated and solved by virtue of differointegral equations. In this subsection we shall solve the problem by the algebraic method developed above. Since the problem is typical and classical for the inverse eigenvalue problem, the algebraic solution of the problem is a good test of our approach.

From the viewpoint of our algebraic approach, the inverse Sturm–Liouville problem is such that the Hamiltonian $\hat{H} = \hat{H}_0 + \hat{V}$, where \hat{H}_0 (the free Hamiltonian or the operator for kinetic energy) is fixed, while the potential \hat{V} is to be determined from the data of the eigensolutions of \hat{H} .

The one-dimensional inverse Sturm–Liouville problem is as follows [16, 17]: for the boundary eigenvalue equations

$$v_n''(x) + [\lambda_n - \hat{q}(x)]v_n(x) = 0 \quad x \in [0, 1] \quad (3.1)$$

$$v_n'(0) = v_n(1) = 0 \quad (3.2)$$

where $v_m(x)$ satisfy the orthonormal relation

$$\int_0^1 v_m(x)v_n(x) dx = \delta_{mn} \quad (3.3)$$

and given the data $\{v_n(0), \lambda_n\}$, construct the potential $\hat{q}(x)$. We apply the method developed in section 2 to solve the problem. From the boundary conditions (3.2), one finds the working basis,

$$|v_p\rangle \equiv |v_p(x)\rangle = \sqrt{2} \cos(2p + \frac{1}{2})\pi x \quad \langle v_p | v_q \rangle = \delta_{pq}. \quad (3.4)$$

In the basis $|v_p\rangle$, we have

$$v_n(x) = |v_n\rangle = \sum_p v_{np} |v_p\rangle = \sqrt{2} \sum_p v_{np} \cos(2p + \frac{1}{2})\pi x \quad (3.5)$$

$$v_n(0) = \sqrt{2} \sum_p v_{np} \quad \sum_n v_{np} v_{nq} = \delta_{pq} \quad (3.6)$$

and

$$\hat{q}(x) = \sum_p q_p \cos(2p + \frac{1}{2})\pi x = \frac{1}{\sqrt{2}} \sum_p q_p |v_p\rangle. \quad (3.7)$$

Where v_{np} or $v_n(0)$ are given and q_p is to be determined. The Hamiltonian is

$$\hat{H} = -\frac{d^2}{dx^2} + \hat{q}(x). \quad (3.8)$$

The matrix elements of \hat{H} can be calculated in two ways. A direct calculation gives

$$H_{pq} = \langle v_p | \hat{H} | v_q \rangle = [(2q + \frac{1}{2})\pi]^2 \delta_{pq} + \frac{1}{2\pi} \sum_r q_r \left\{ \frac{1}{2(r+p-q) + \frac{1}{2}} + \frac{1}{2(r-p+q) + \frac{1}{2}} - \frac{1}{2(r+p+q) + \frac{3}{2}} - \frac{1}{2(r-p-q) - \frac{1}{2}} \right\}. \quad (3.9)$$

From the eigenrepresentation of \hat{H} ,

$$\hat{H} = \sum_n |v_n\rangle \lambda_n \langle v_n| \quad (3.10)$$

we have

$$H_{pq} = \sum_n \lambda_n v_{np} v_{nq}. \quad (3.11)$$

Combining equations (3.9) and (3.11), one obtains

$$[(2q + \frac{1}{2})\pi]^2 \delta_{pq} + \sum_r q_r D_{prq} = \sum_n \lambda_n v_{np} v_{nq} \quad (3.12)$$

where

$$D_{prq} = \frac{1}{2\pi} \left\{ \frac{1}{2(r+p-q) + \frac{1}{2}} + \frac{1}{2(r-p+q) + \frac{1}{2}} - \frac{1}{2(r+p+q) + \frac{3}{2}} - \frac{1}{2(r-p-q) - \frac{1}{2}} \right\}. \quad (3.13)$$

Summing equation (3.12) over q , we obtain

$$\sum_r C_{prq} = \sum_{nq} \lambda_n v_{np} v_{nq} - [(2p + \frac{1}{2})\pi]^2 \quad (3.14)$$

where

$$C_{pr} = \sum_q D_{prq}. \quad (3.15)$$

The solution is

$$q_p = \sum_r C_{pr}^{-1} \left\{ \sum_{nq} \lambda_n v_{nr} v_{nq} - [(2r + \frac{1}{2})\pi]^2 \right\}. \quad (3.16)$$

From equations (3.12) and (3.16), we obtain a set of nonlinear equations for v_{np} ,

$$\{[(2p + \frac{1}{2})\pi]^2 - \lambda_n\} v_{np} + \sum_{qr} D_{prq} v_{nq} \sum_s C_{rs}^{-1} \left\{ \frac{1}{\sqrt{2}} \sum_m \lambda_m v_{ms} v_m(0) - [(2s + \frac{1}{2})\pi]^2 \right\} = 0 \quad (3.17)$$

which are homogeneous because of the orthonormal conditions of v_{np} (equation (3.6)).

Equations (3.7), (3.16) and (3.17) constitute a set of basic equations for the one-dimensional inverse Sturm–Liouville problem. If both eigenvalues and eigenvectors are given, the information is sufficient to construct the potential just using equations (3.16) and (3.7). If only λ_n and $v_n(0)$ are known, one has to resort to the nonlinear equation (3.17). This is the price paid for less information.

Example. Given $\lambda_n = [(2n + \frac{1}{2})\pi]^2$ and $v_n(0) = \sqrt{2}$, calculate $\hat{q}(x)$. Multiplying equation (3.17) with v_{np} and summing over n and p , we have

$$\sum_{pr} D_{prp} \sum_s C_{rs}^{-1} \sum_m [(2m + \frac{1}{2})\pi]^2 (v_{ms} - \delta_{ms}) = 0. \quad (3.18)$$

Since $\sum_p D_{prp} \neq 0$, $\det C^{-1} \neq 0$, and $[(2m + \frac{1}{2})\pi]^2 > 0$, we have the solution

$$v_{ms} = \delta_{ms} \quad \text{and} \quad v_m(0) = \sqrt{2}. \quad (3.19)$$

From equation (3.16), we obtain $q_p = 0$ and $\hat{q}(x) = 0$.

3.2. Quantum regular spectrum

We consider the inverse problems for regular quantum spectra in the $su(2)$ and the HW representations.

3.2.1. Finite-dimensional Hilbert space. $su(2)$ representation.

Example 1. Given $E_m = m$ and $U_{mn} = \delta_{mn}$, construct \hat{H} . From equation (2.18) and as j is very large, we have

$$\begin{aligned} h_p &= \frac{1}{2j+1} \sum_m m \exp(-i\alpha_p m) = \frac{1}{2j+1} i \frac{\partial}{\partial \alpha_p} \sum_m \exp(-i\alpha_p m) \\ &= \frac{2\pi}{2j+1} i \frac{\partial}{\partial \alpha_p} \delta(\alpha_p) \quad j \rightarrow \infty. \end{aligned} \quad (3.20)$$

\hat{H}_0 can be obtained from equation (2.15),

$$\begin{aligned} \hat{H}_0 &= \sum_p \frac{2\pi}{2j+1} i \frac{\partial}{\partial \alpha_p} \delta(\alpha_p) \exp(i\alpha_p \hat{J}_z) \\ &= \int d\alpha_p i \frac{\partial}{\partial \alpha_p} \delta(\alpha_p) \exp(i\alpha_p \hat{J}_z) = \hat{J}_z \quad j \rightarrow \infty. \end{aligned} \tag{3.21}$$

From equations (2.22) and (2.27), one has

$$\begin{aligned} D_{pq} &= \frac{1}{(2j+1)^2} \sum_{k_1 k_2} \left(\frac{j^{k_1+k_2}}{d_{k_1 k_2}^{(j)}(\theta)} \sum_m \exp(im\theta) \Delta_{k_1 m} \Delta_{k_2 m} \right) \exp(ik_1 \alpha_p + ik_2 \alpha_q) \\ &= \frac{1}{(2j+1)^2} \sum_{k_1 k_2} \exp(ik_1 \alpha_p + ik_2 \alpha_q) = \delta_{p,0} \delta_{q,0}. \end{aligned} \tag{3.22}$$

From equations (2.19) and (2.28), we obtain $\hat{U} = 1$, and $\hat{H} = \hat{J}_z$.

Example 2. Given $H_{mn} = m\delta_{mn}$, construct \hat{H} .

We use the polynomial representation. Since $H_{mm} = jT_1(m/j)$, as j is very large, we have from equation (2.47)

$$\begin{aligned} h_p &= \frac{j(2-\delta_{p0})}{(2j+1)\pi} \sum_m T_1\left(\frac{m}{j}\right) T_p\left(\frac{m}{j}\right) \left[1 - \left(\frac{m}{j}\right)^2\right]^{-1/2} \\ &= \frac{j(2-\delta_{p0})}{\pi} \int_{-1}^1 dx T_1(x) T_p(x) (1-x^2)^{-1/2} = j\delta_{p,1} \end{aligned} \tag{3.23}$$

while equation (2.44) yields $\hat{H}_0 = jT_1(\hat{J}_z/j) = \hat{J}_z$. In equation (2.48), since the coefficient determinant is non-zero, $H_{mn} = 0$ ($m \neq n$) yields the vanishing solution $D_{pq} = 0$. Thus $\hat{H} = \hat{H}_0 = \hat{J}_z$.

3.2.2. Infinite-dimensional Hilbert space. HW representation.

Example 1. Given $E_m = m$ and $U_{mn} = \delta_{mn}$, construct \hat{H} .

From equation (2.35) we have

$$h_p = \lim_{N \rightarrow \infty} \frac{1}{2(N+1)} i \frac{\partial}{\partial \alpha_p} \sum_m^N \exp(-i\alpha_p m) = \lim_{N \rightarrow \infty} \frac{2\pi}{2(N+1)} i \frac{\partial}{\partial \alpha_p} \delta(\alpha_p) \tag{3.24}$$

while equation (2.32) yields

$$\begin{aligned} \hat{H}_0 &= \lim_{N \rightarrow \infty} \frac{2\pi}{2(N+1)} \sum_p \left(i \frac{\partial}{\partial \alpha_p} \delta(\alpha_p) \exp(i\alpha_p \hat{n}) + \text{HC} \right) \\ &= \frac{1}{2} \int d\alpha_p \left(i \frac{\partial}{\partial \alpha_p} \delta(\alpha_p) \exp(i\alpha_p \hat{n}) + \text{HC} \right) = \frac{1}{2} (\hat{n} + \hat{n}) = \hat{n}. \end{aligned} \tag{3.25}$$

D_{rs} can be calculated from equation (2.41),

$$\begin{aligned} D_{rs} &= \frac{1}{2\pi} \sum_m \int dk \langle \psi_{k+r} | m \rangle \langle m | \psi_k \rangle \exp(-isk) = \frac{1}{2\pi} \int dk \langle \psi_{k+r} | \psi_k \rangle \exp(-isk) \\ &= \frac{1}{2\pi} \int dk \delta(r) \exp(-isk) = \delta(r) \delta(s). \end{aligned} \tag{3.26}$$

From equation (2.36), one has

$$\hat{U} = \int dr ds \delta(r) \delta(s) \exp(ir \hat{x}) \exp(is \hat{p}) = 1. \tag{3.27}$$

Hence $\hat{H} = \hat{U} \hat{H}_0 \hat{U}^{-1} = \hat{n} = \frac{1}{2} (\hat{p}^2 + \hat{x}^2) - \frac{1}{2}$.

Example 2. Given $H_{mn} = m\delta_{mn}$, construct \hat{H} .

Working in the polynomial representation, we rewrite $H_{nn} = n = (N/2)[T_1((2n - N)/N) + T_0]$ and substitute it in equation (2.53)

$$\begin{aligned} h_p &= \lim_{N \rightarrow \infty} \frac{N(2 - \delta_{p0})}{2(N+1)\pi} \sum_n \left[T_1 \left(\frac{2n - N}{N} \right) + T_0 \right] T_p \left(\frac{2n - N}{N} \right) \left[1 - \left(\frac{2n - N}{N} \right)^2 \right]^{-1/2} \\ &= \lim_{N \rightarrow \infty} \frac{N(2 - \delta_{p0})}{2\pi} \int_{-1}^1 dx [T_1(x) + T_0(x)] T_p(x) (1 - x^2)^{-1/2} \\ &= \lim_{N \rightarrow \infty} \frac{N}{2} (\delta_{p,1} + \delta_{p,0}). \end{aligned} \quad (3.28)$$

From equation (2.50), we obtain

$$\begin{aligned} \hat{H}_0 &= \lim_{N \rightarrow \infty} \frac{N}{2} \left[T_1 \left(\frac{2\hat{n} - N}{N} \right) + T_0 \left(\frac{2\hat{n} - N}{N} \right) \right] \\ &= \lim_{N \rightarrow \infty} \frac{N}{2} \left(\frac{2\hat{n} - N}{N} + 1 \right) = \hat{n}. \end{aligned} \quad (3.29)$$

Since in equation (2.54) the coefficient determinant is non-zero, $H_{mn} = 0$ ($n \neq m$) yields the solution $D_{pq} = 0$. Therefore, we finally obtain $\hat{H} = \hat{H}_0 = \hat{n}$.

3.3. Quantum irregular spectrum

In this subsection, we shall employ the information contained in this paper to study the problem of quantum chaos. We start with the following question: given a set of eigenenergies E_n and eigenstates ψ_n with GOE (Gaussian orthogonal ensemble) [12] statistics built in, is it possible to construct a Hamiltonian within some dynamical algebra to reproduce the data? A positive answer can be obtained with the help of the preceding results. Since the data E_n and the data ψ_n can be used to construct the $\hat{H}_0(\hat{h}_i)$ and the $\hat{U}(\hat{X}_\alpha)$, respectively, the Hamiltonian $\hat{H} = \hat{U}\hat{H}_0\hat{U}^{-1}$ is the required one that can reproduce the data. From a practical point of view, since a physical data set is usually finite, the construction of \hat{H} can be conducted in a finite-dimensional Hilbert space, the calculability of which is limited merely by the capacity of modern computers.

The results obtained in section 2 provide some new insight into the problem of quantum chaos. From the above discussion we know that, the information of the energy spectrum is related to an integrable Hamiltonian \hat{H}_0 which generates a set of regular eigenstates with good quantum numbers (n_i) [15], while the information of the eigenstates is connected with a unitary transformation which destroys the good quantum numbers and makes the wavefunctions more complicated. This result indicates that as only eigenenergies are concerned, even an integrable Hamiltonian [15] can yield a GOE energy spectrum. This contradicts the conventional point of view that an integrable Hamiltonian cannot have a GOE energy spectrum. The information of the eigenfunctions on the other hand is more essential to construct a non-integrable Hamiltonian, since the \hat{U} which is related to the wavefunctions destroys good quantum numbers and makes the system non-integrable. The above fact tells us that the information of the energy spectrum alone is insufficient to make a judgement about the chaoticity of a quantum system, while the information of the eigenstates is more important in this respect. Here one finds a kind of classical-quantum correspondence in the chaotic case: the classical chaoticity is related to the chaotic trajectories, while the quantum chaoticity is connected with the irregular eigenwavefunctions.

The information provided in this paper also helps us to understand the results obtained in our recent study of quantum chaos. In [18] we constructed a one-dimensional $SU(2)$ model whose energy spectrum can show both GOE and Poisson statistics, as the parameters were properly chosen. Since the common expectation is that a one-dimensional integrable system should not show GOE statistics [19], and Poisson statistics in conservative systems are usually found for at least two dimensions [20], this result is remarkable and deserves further investigation. At first glance this result is astonishing, but it is not difficult to understand from the above results. In section 2 we have shown in detail that a one-dimensional Hamiltonian can be constructed from any type of input data E_n and ψ_n including, of course, GOE type or Poisson type. This implies that the one-dimensional $SU(2)$ Hamiltonian can show GOE or Poisson statistics of its eigenspectrum if it is properly constructed. This is a new insight into the one-dimensional problem. The question is how a relatively simple Hamiltonian can produce very complicated GOE statistics. The inverse method developed in this paper unfortunately cannot answer this question. However, the level dynamics reformulated in [18] can shed some light on this difficult problem: if a relatively simple Hamiltonian has a large number of strong avoided level crossings during the change of its perturbation strength, the fluctuation in both E_n and ψ_n will be set in and the system could exhibit GOE statistics.

4. Discussion

In this paper, we have presented an algebraic approach to the inverse eigenvalue problem for a quantum system with a dynamical group. In comparison with the classical Sturm–Liouville inverse eigenvalue problem, three points in our approach are different and deserve remarking on. (i) Instead of recovery of a potential, our task is to reconstruct a whole Hamiltonian. Thus the recovery of a potential is just a special case. (ii) Rather than considering a general Hamiltonian, a class of physically relevant Hamiltonians with dynamical group structures is studied here. Specifically speaking, the Hamiltonian investigated in this paper is a nonlinear function of the generators of a certain kind of dynamical algebras and an object of the corresponding enveloping algebra. (iii) Since a physically relevant algebra usually dictates a special structure of a Hilbert space and its representation provides a basis for the Hilbert space, the inverse eigenvalue problem formulated in this basis becomes an algebraic problem. Thus our algebraic approach is complementary to the conventional differential–integral approach where the representation basis is just the Dirac delta function.

Just as in the conventional approach to the inverse problem, in this paper the one-dimensional problem is solved also with a great detail for both finite and infinite dimensional Hilbert spaces, and the analytical expressions for the expansion coefficients of the Hamiltonian are given. For the multidimensional cases, the generalization presents little difficulty.

As applications, our approach has been tested first by the classical Sturm–Liouville inverse eigenvalue problem and then by several simple examples where the analytical results can be obtained. For more complicated spectra, the recent new results of the $SU(2)$ model are discussed and explained.

For the inverse problem in general, several questions deserve discussion. The first question is the existence and uniqueness of the solution. Since our method is essentially a constructive approach and the expression of the solution is given explicitly, the existence problem is of course solved. As to the uniqueness, there are two aspects to be investigated:

(i) The uniqueness of \hat{H} in a subspace. Since the Hamiltonian constructed in different bases has different expressions but reproduces the same eigensolution in the subspace, it is unique by definition.

(ii) The uniqueness of \hat{H} in the whole Hilbert space. Usually, the Hamiltonians constructed in a subspace and expanded in terms of different bases are not equivalent and will yield different eigensolutions in an enlarged space. To obtain a unique solution in the whole Hilbert space, one needs either to work in a very large Hilbert space that approaches the whole Hilbert space in the limit or to work in the whole Hilbert space from the beginning. In section 3 (applications), we did that and obtained the unique solution applicable in the whole Hilbert space.

Another interesting problem is related to the power of the inverse theory. There are two opposite sides in the inverse problem. On one hand, one has numerical input data (ψ_n and E_n), which is the phenomenological aspect of the problem. The quantity of information contained in the input data is very large. On the other, one has a Hamiltonian \hat{H} which represents the natural law governing the phenomenon. The quantity of information contained in \hat{H} (i.e. the number of parameters contained in \hat{H}) is less. The line of reasoning in the direct problem is from the natural law to its governing phenomenon. In the course of solving the direct problem, the relevant information is expanded. Logically this is a kind of deduction. The line of reasoning in the inverse problem is the opposite. It goes from the phenomenon to its underlying law. The information is compressed during the process of solution. Logically this is a kind of induction. From the above discussion we see that the method of the inverse problem is a tool that helps to compress information and discover natural laws from the phenomenological input.

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