Analytically solvable quantum Hamiltonians and relations to orthogonal polynomials

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Abstract

Quantum systems consisting of a linear chain of n harmonic oscillators coupled by a quadratic nearest-neighbour interaction are considered. We investigate when such a system is analytically solvable, in the sense that the eigenvalues and eigenvectors of the interaction matrix have analytically closed expressions. This leads to a relation with Jacobi matrices of systems of discrete orthogonal polynomials. Our study is first performed in the case of canonical quantization. Then we consider these systems under Wigner quantization, leading to solutions in terms of representations of Lie superalgebras. Finally, we show how such analytically solvable Hamiltonians also play a role in another application, that of spin chains used as communication channels in quantum computing. In this context, the analytic solvability leads to closed form expressions for certain transition amplitudes.

1 Introduction

One-dimensional systems with a nearest-neighbour interaction have received a lot of attention, especially those that are still exactly solvable. Among the most famous, we mention the Toda system [1] and the Calogero-Sutherland-Moser models [2–4]. In this context, the emphasis is on mathematical aspects such as integrability and the underlying algebraic structures.

Also the quantum versions of many of these systems or models were investigated from various points of view during the last decades [5,6]. In such quantum systems, the emphasis – from the physics point of view – is on a construction of ground wave states, formulae for the excitation spectrum, a description of stationary states, etc.

In the present paper we consider quantum systems consisting of a one-dimensional chain of particles with a nearest-neighbour interaction that is

quadratic in the position operators. The Hamiltonian of such a system will be written as

$$\hat{H} = \sum_{r=1}^{n} \left(\frac{\hat{p}_r^2}{2m} + \frac{m\omega^2}{2} \hat{q}_r^2 \right) - \frac{cm}{2} \sum_{r=1}^{n-1} \gamma_r \hat{q}_r \hat{q}_{r+1}. \tag{1}$$

This quantum system consists of a string or chain of n identical harmonic oscillators, each having the same mass m and natural frequency ω. As usual, the position and momentum operators for the rth oscillator are given by $\hat{q}_r$ and $\hat{p}_r$; more precisely $\hat{q}_r$ measures the displacement of the rth mass point with respect to its equilibrium position. The (positive) constants γ_r refer to the interaction strength between oscillators r and $(r+1)$, and c is an overall coupling constant. In order to have a physical meaning, the interaction matrix (see later) related to (1) should be positive definite.

Hamiltonians of the form (1) are always numerically solvable. The purpose of this paper is to study cases where a Hamiltonian of this type is analytically solvable, i.e. when the eigenvalues of $\hat{H}$ are known in analytically closed form. As we shall see, one example is

$$\hat{H}_K = \sum_{r=1}^{n} \left(\frac{\hat{p}_r^2}{2m} + \frac{m\omega^2}{2} \hat{q}_r^2 \right) - \frac{cm}{2} \sum_{r=1}^{n-1} \sqrt{r(n-r)} \, \hat{q}_r \hat{q}_{r+1}. \tag{2}$$

A Hamiltonian of the form (1) is determined by its interaction matrix, which is tridiagonal. By identifying this tridiagonal interaction matrix with the Jacobi matrix of a set of discrete orthogonal polynomials, we are able to derive new examples of analytically solvable Hamiltonians. This method is outlined in Section 2, where the example (2) is discussed as well.

As expected, such an analysis is carried out in the case that the position and momentum operators are self-adjoint, and satisfy the canonical commutation relations (CCRs)

$$[\hat{q}_r, \hat{q}_s] = 0, \quad [\hat{p}_r, \hat{p}_s] = 0, \quad [\hat{q}_r, \hat{p}_s] = i\hbar\delta_{rs} \quad (r, s = 1, \ldots, n). \tag{3}$$

More interestingly, the Hamiltonians of this form can also be solved as a Wigner quantum system. In that case, the CCRs are *not* required, but instead some more general quantization conditions are imposed for the operators $\hat{q}_r$ and $\hat{p}_r$. The analysis of this is performed in Section 3, where we show that the new quantization conditions lead to a relation with Lie superalgebras.

Finally, we consider a quantum system that is in nature completely different from the ones we have described so far, but which is also determined by an interaction matrix. Such systems consist of a chain of fermions (spin $1/2$ particles) with a nearest-neighbour hopping interaction, subject to a non-uniform magnetic field. It will be clear that the solutions of such systems are closely related to those of the earlier described oscillator systems. This topic will be discussed in Section 4.

The purpose of this contribution is to give a review of the connection between analytically solvable quantum Hamiltonians and (discrete) orthogonal polynomials, the Wigner quantization of such Hamiltonians, and to indicate how the

same type of Hamiltonians appear in a different context where the analytical solvability plays again an important role. The first topic has been discussed in detail in [7], where more examples of analytically solvable quantum Hamiltonians are given. The Wigner quantization is only briefly explained here; for more details, the reader is referred to [8].

2 Oscillators with a nearest-neighbour interaction

2.1 General method

The Hamiltonian (1) can be written in matrix form and is determined by an interaction matrix M:

$$
\hat{H} = \frac{1}{2m} \begin{pmatrix} \hat{p}_1^\dagger & \cdots & \hat{p}_n^\dagger \end{pmatrix} \begin{pmatrix} \hat{p}_1 \\ \vdots \\ \hat{p}_n \end{pmatrix}
$$

$$
+ \frac{m}{2} \begin{pmatrix} \hat{q}_1^\dagger & \cdots & \hat{q}_n^\dagger \end{pmatrix} (\omega^2 I + cM) \begin{pmatrix} \hat{q}_1 \\ \vdots \\ \hat{q}_n \end{pmatrix}, \tag{4}
$$

where in this case

$$
M = \begin{pmatrix} 0 & -\gamma_1/2 & & \\ -\gamma_1/2 & 0 & \ddots & \\ & \ddots & \ddots & -\gamma_{n-1}/2 \\ & & -\gamma_{n-1}/2 & 0 \end{pmatrix}. \tag{5}
$$

More generally, assume that M is a *real and symmetric* matrix, and that $\omega^2 I + cM$ is a positive definite matrix [9, 10]. A general method to deal with such Hamiltonians was described in [9, section 2.1]. Since M is real and symmetric, the spectral theorem [11] implies

$$
M = UDU^T \tag{6}
$$

where

$$
D = \mathrm{diag}(\lambda_1, \lambda_2, \ldots, \lambda_n), \tag{7}
$$

$$
UU^T = U^T U = I. \tag{8}
$$

The entries of the diagonal matrix D are the (real) eigenvalues λ_i of M, in some order, and the columns of the real orthogonal matrix U are eigenvectors of M (in the same order); U^T stands for the transpose of U.

Introducing new operators (the so-called normal coordinates and momenta) as follows:

$$
\begin{pmatrix} \hat{Q}_1 \\ \vdots \\ \hat{Q}_n \end{pmatrix} = U^T \begin{pmatrix} \hat{q}_1 \\ \vdots \\ \hat{q}_n \end{pmatrix}, \qquad \begin{pmatrix} \hat{P}_1 \\ \vdots \\ \hat{P}_n \end{pmatrix} = U^T \begin{pmatrix} \hat{p}_1 \\ \vdots \\ \hat{p}_n \end{pmatrix}, \tag{9}
$$

the Hamiltonian (4) reads

$$\hat{H} = \frac{1}{2m} \begin{pmatrix} \hat{P}_1^\dagger & \cdots & \hat{P}_n^\dagger \end{pmatrix} \begin{pmatrix} \hat{P}_1 \\ \vdots \\ \hat{P}_n \end{pmatrix}$$

$$+ \frac{m}{2} \begin{pmatrix} \hat{Q}_1^\dagger & \cdots & \hat{Q}_n^\dagger \end{pmatrix} (\omega^2 I + cD) \begin{pmatrix} \hat{Q}_1 \\ \vdots \\ \hat{Q}_n \end{pmatrix}$$

$$= \frac{1}{2m} \sum_{j=1}^n \hat{P}_j^2 + \frac{m}{2} \sum_{j=1}^n (\omega^2 + c\lambda_j)\hat{Q}_j^2. \tag{10}$$

By the transformation (9), the new operators also satisfy the canonical commutation relations:

$$[\hat{Q}_j, \hat{Q}_k] = 0, \quad [\hat{P}_j, \hat{P}_k] = 0, \quad [\hat{Q}_j, \hat{P}_k] = i\hbar\delta_{jk} \quad (j, k = 1, \ldots, n). \tag{11}$$

In (10), the values of $\omega^2 + c\lambda_j$ are all positive since the interaction matrix $\omega^2 I + cM$ is assumed to be positive definite. So one can introduce

$$\omega_j = \sqrt{\omega^2 + c\lambda_j} \tag{12}$$

and write

$$\hat{H} = \frac{1}{2m} \sum_{j=1}^n \hat{P}_j^2 + \frac{m}{2} \sum_{j=1}^n \omega_j^2 \hat{Q}_j^2. \tag{13}$$

This expression is just like the Hamiltonian of an n-dimensional non-isotropic oscillator, so we can use the commonly known method for its solution [12, 13]. Introducing boson operators

$$a_j^\pm = \sqrt{\frac{m\omega_j}{2\hbar}}\hat{Q}_j \mp \frac{i}{\sqrt{2\hbar m\omega_j}}\hat{P}_j, \tag{14}$$

these satisfy

$$[a_j^-, a_k^-] = [a_j^+, a_k^+] = 0, \qquad [a_j^-, a_k^+] = \delta_{jk}, \qquad (j, k = 1, \ldots, n) \tag{15}$$

and $\hat{H}$ can be written as

$$\hat{H} = \sum_{j=1}^n \frac{\hbar\omega_j}{2}\{a_j^+, a_j^-\} = \sum_{j=1}^n \frac{\hbar\omega_j}{2}(2a_j^+ a_j^- + 1). \tag{16}$$

Furthermore,

$$[\hat{H}, a_j^\pm] = \pm\hbar\omega_j\, a_j^\pm \qquad (j = 1, \ldots, n). \tag{17}$$

So if we assume that there is a lowest $\hat{H}$-eigenvalue (lowest energy), say for the state $|0\rangle$, then we have the usual n-boson Fock space in which the action of $\hat{H}$ is diagonal. The vacuum vector $|0\rangle$ satisfies

$$\langle 0|0\rangle = 1, \qquad a_j^- |0\rangle = 0; \tag{18}$$

the other (orthogonal and normalized) basis vectors are then defined by

$$|k_1, \ldots, k_n\rangle = \frac{(a_1^+)^{k_1} \ldots (a_n^+)^{k_n}}{\sqrt{k_1! \ldots k_n!}} |0\rangle, \qquad (k_j = 0, 1, \ldots). \tag{19}$$

The spectrum of $\hat{H}$ is now determined by

$$\hat{H}|k_1, \ldots, k_n\rangle = \sum_{j=1}^{n} \hbar\omega_j(k_j + \frac{1}{2}) \, |k_1, \ldots, k_n\rangle. \tag{20}$$

This analysis is well known, and it seems to indicate that a Hamiltonian of the form (4) with a general interaction matrix M is exactly solvable as a quantum system. Note, however, that the solution we have described involves also a *numerical process*, namely the determination of the eigenvalues and eigenvectors of M in (7) and (8). We shall say that the Hamiltonian $\hat{H}$ is *analytically solvable* if we have an analytically closed expression for the eigenvalues and eigenvectors of M, for arbitrary n.

One classical example of an analytically solvable Hamiltonian is the case where the couplings of neighbouring oscillators are identical and described by Hooke's law. In that case, the interaction matrix M has constant entries on the first diagonal below and above the main diagonal [14, 15]. In the following subsection, we shall present another example of an analytically solvable Hamiltonian.

2.2 Krawtchouk interaction

We shall first describe some properties of Krawtchouk polynomials, and then relate their Jacobi matrix to a solvable Hamiltonian.

For a fixed positive integer parameter N and a real parameter p ($0 < p < 1$), the Krawtchouk polynomial of degree i ($i = 0, 1, \ldots, N$) in the variable x is defined by [16, 17]

$$K_i(x) \equiv K_i(x; p, N) = {}_2F_1\left(\begin{matrix} -x, -i \\ -N \end{matrix} ; \frac{1}{p} \right). \tag{21}$$

Herein, ${}_2F_1$ is the usual Gauss hypergeometric series [18]

$$ {}_2F_1\left(\begin{matrix} a, b \\ c \end{matrix} ; z \right) = \sum_{k=0}^{\infty} \frac{(a)_k (b)_k}{(c)_k} \frac{z^k}{k!}. \tag{22}$$

In (21), the series is terminating because one of the numerator parameters is a negative integer. Note that in (22) we use the notation of the raising factorial,

which can also be rewritten by means of a (generalized) binomial coefficient:

$$(a)_k = a(a+1)\cdots(a+k-1) = (-1)^k \binom{-a}{k} k!$$

The Krawtchouk polynomials satisfy a discrete orthogonality relation of the form

$$\sum_{x=0}^{N} w(x) K_i(x) K_j(x) = d_i \delta_{ij}, \tag{23}$$

where $w(x)$ is a weight function in x and d_i is a function depending on i:

$$w(x) = \binom{N}{x} p^x (1-p)^{N-x} \qquad (x = 0, 1, \ldots, N); \tag{24}$$

$$d_i = \frac{1}{\binom{N}{i}} \left(\frac{1-p}{p}\right)^i. \tag{25}$$

Recall that the recurrence relation for Krawtchouk polynomials is given by

$$-x K_i(x) = i(1-p) K_{i-1}(x) - \left[p(N-i) + i(1-p)\right] K_i(x) + p(N-i) K_{i+1}(x). \tag{26}$$

For future purposes we will however be interested in an orthonormality condition, so we define the orthonormal Krawtchouk functions by

$$\tilde{K}_i(x) \equiv \tilde{K}_i(x; p, N) = \frac{\sqrt{w(x)}\, K_i(x)}{\sqrt{d_i}}, \qquad i = 0, 1, 2, \ldots, N. \tag{27}$$

Now we can state the following property [7]:

Lemma 1 *Let M_K be the tridiagonal $(N+1) \times (N+1)$-matrix*

$$M_K = \begin{pmatrix} F_0 & -E_1 & 0 & & \\ -E_1 & F_1 & -E_2 & \ddots & \\ 0 & -E_2 & F_2 & \ddots & 0 \\ & \ddots & \ddots & \ddots & -E_N \\ & & 0 & -E_N & F_N \end{pmatrix}, \tag{28}$$

where

$$E_i = \sqrt{p(1-p)}\sqrt{i(N-i+1)}, \qquad F_i = Np + (1-2p)i, \tag{29}$$

and let U be the $(N+1) \times (N+1)$-matrix with matrix elements

$$U_{ij} = \tilde{K}_i(j) = \left[\binom{N}{i}\binom{N}{j} p^{i+j}(1-p)^{N-i-j}\right]^{1/2} \sum_{k=0}^{\min(i,j)} \frac{\binom{i}{k}\binom{j}{k}}{\binom{N}{k}} \left(-\frac{1}{p}\right)^k, \tag{30}$$

where $i, j = 0, 1, \ldots, N$. Then

$$UU^T = U^T U = I \qquad and \qquad M_K = UDU^T \tag{31}$$

where $D = diag(0, 1, 2\ldots, N)$.

For a proof, see [7]. The main ingredient of the proof is the recurrence relation for the $\tilde{K}_i$:

$$x\tilde{K}_i(x) = -E_i\,\tilde{K}_{i-1}(x) + F_i\,\tilde{K}_i(x) - E_{i+1}\,\tilde{K}_{i+1}(x). \tag{32}$$

Now have a good candidate interaction matrix M_K. In order to correspond to systems of the form (1), however, the diagonal entries F_i of M_K should be constants (i.e. independent of i). We see from (29) that this is the case for $p = 1/2$. This leads us to the following Hamiltonian "with Krawtchouk interaction":

$$\hat{H}_K = \sum_{r=1}^{n}\left(\frac{\hat{p}_r^2}{2m} + \frac{m\omega^2}{2}\hat{q}_r^2\right) - \frac{cm}{2}\sum_{r=1}^{n-1}\sqrt{r(n-r)}\,\hat{q}_r\hat{q}_{r+1}. \tag{33}$$

This can indeed be written in matrix form:

$$\hat{H}_K = \frac{1}{2m}\left(\begin{array}{ccc} \hat{p}_1^\dagger & \cdots & \hat{p}_n^\dagger \end{array}\right)\left(\begin{array}{c} \hat{p}_1 \\ \vdots \\ \hat{p}_n \end{array}\right)$$

$$+ \frac{m}{2}\left(\begin{array}{ccc} \hat{q}_1^\dagger & \cdots & \hat{q}_n^\dagger \end{array}\right)\left((\omega^2 - \frac{c(n-1)}{2})I + cM_K\right)\left(\begin{array}{c} \hat{q}_1 \\ \vdots \\ \hat{q}_n \end{array}\right), \tag{34}$$

where M_K is the matrix (28) with $N = n - 1$ and $p = 1/2$. Using the explicitly known spectral decomposition, given in Lemma 1, and following the general procedure described in the previous subsection, one introduces here the following quantities ($j = 1, 2, \ldots, n$):

$$\omega_j = \sqrt{\omega^2 - \frac{c(n-1)}{2} + c(j-1)} = \sqrt{\omega^2 - \frac{c}{2}(n-2j+1)}. \tag{35}$$

The interaction matrix $(\omega^2 - \frac{c(n-1)}{2})I + cM_K$ is positive definite if all quantities under the square root symbol are positive. Since c (and ω^2) is positive, $\omega^2 - \frac{c(n-1)}{2} + c(j-1)$ ($j = 1, 2, \ldots, n$) is an increasing sequence as j increases. So this condition leads to $c < 2\omega^2/(n-1)$, or the "coupling strength" should be sufficiently small. Now we have:

Proposition 2 *The Hamiltonian $\hat{H}_K$ given by (33) is analytically solvable. The explicit spectrum of H_K follows from (20):*

$$\hat{H}_K|k_1,\ldots,k_n\rangle = \sum_{j=1}^{n}\hbar\omega_j(k_j + \frac{1}{2})\,|k_1,\ldots,k_n\rangle, \tag{36}$$

where the constants ω_j are given by $\omega_j = \sqrt{\omega^2 - c(n-2j+1)/2}$.

From this example, it should be clear that the general procedure worked out here for Krawtchouk polynomials works in general for discrete orthogonal polynomials. In order to find other interesting examples, one can go through the list

of discrete orthogonal polynomials [16, 17] and their q-analogues. The basic restriction, in order to have Hamiltonians of the form (1), is that the diagonal elements in the interaction matrix are constant (for specific values of the parameters). This analysis has been done in [7], leading to only two more such cases: the Hahn polynomials with $\beta = \alpha$ and the dual q-Krawtchouk polynomials with $\bar{c} = -1$. For further details of these Hamiltonians and properties of their spectra, the reader is referred to [7].

3 Wigner's quantization procedure and relations with Lie superalgebras

We shall now consider an alternative quantization of the Hamiltonians introduced in the previous section, known as Wigner quantization. Eugene Wigner [19] was the first to realize that one does not need to assume the CCRs in order to find operators that satisfy Hamilton's equations (in operator form) and the equations of Heisenberg simultaneously. In Wigner quantization, one does not assume the CCRs. Instead, one expresses the compatibility of Hamilton's equations and the Heisenberg equations. This leads to compatibility conditions (CCs) that are more general than the CCRs [20]. In other words, the canonical quantization is a particular case of Wigner quantization.

Let us rewrite the Hamiltonian with a general interaction matrix (4) as

$$
\begin{aligned}
\hat{H} &= \frac{1}{2m} \begin{pmatrix} \hat{p}_1^\dagger & \cdots & \hat{p}_n^\dagger \end{pmatrix} \begin{pmatrix} \hat{p}_1 \\ \vdots \\ \hat{p}_n \end{pmatrix} + \frac{m}{2} \begin{pmatrix} \hat{q}_1^\dagger & \cdots & \hat{q}_n^\dagger \end{pmatrix} A \begin{pmatrix} \hat{q}_1 \\ \vdots \\ \hat{q}_n \end{pmatrix} \\
&= \frac{1}{2m} \sum_{r=1}^n \hat{p}_r^2 + \frac{m}{2} \sum_{r,s=1}^n A_{rs} \hat{q}_r \hat{q}_s.
\end{aligned}
\tag{37}
$$

So herein $A = \omega^2 I + cM$, and the matrix $A = (A)_{1 \le r,s \le n}$ is again assumed to be real, symmetric and positive definite.

Let us now move to the Wigner quantization procedure. The operator form of Hamilton's equations is

$$
\dot{\hat{p}}_r = -\frac{\partial \hat{H}}{\partial \hat{q}_r}, \qquad \dot{\hat{q}}_r = \frac{\partial \hat{H}}{\partial \hat{p}_r},
\tag{38}
$$

and the Heisenberg equations read

$$
\dot{\hat{p}}_r = \frac{i}{\hbar}[\hat{H}, \hat{p}_r], \qquad \dot{\hat{q}}_r = \frac{i}{\hbar}[\hat{H}, \hat{q}_r].
\tag{39}
$$

Their equivalence results in the following compatibility conditions (CCs):

$$
\begin{aligned}
[\hat{H}, \hat{q}_r] &= -\frac{i\hbar}{m} \hat{p}_r, \\
[\hat{H}, \hat{p}_r] &= i\hbar m \sum_{s=1}^n A_{rs} \hat{q}_s,
\end{aligned}
\tag{40}
$$

with $r = 1, 2, \ldots, n$. We are now looking for operator solutions for $\hat{q}_r$ and $\hat{p}_r$ satisfying the compatibility conditions (40), with Hamiltonian (37). Since the matrix A is real and symmetric, we can again apply the spectral theorem and write

$$A = U D_A U^T. \tag{41}$$

Note that, with $A = \omega^2 I + cM$ as in the previous section, the orthogonal matrix U is the same as for M, and $D_A = \omega^2 I + cD$, with D the diagonalization of M. So D_A is diagonal with the real and positive eigenvalues μ_j $(j = 1, \ldots, n)$ of A as diagonal elements. Using the orthogonal matrix U, one introduces once again normal coordinates and momenta $\hat{Q}_j$ and $\hat{P}_j$ by the same transformation (9). The difference is of course that in the current case the new operators do *not* satisfy the canonical commutation relations, since these are not required for the $\hat{q}_j$ and $\hat{p}_j$ either. In function of the normal coordinates and momenta, the Hamiltonian (37) can be rewritten as

$$\hat{H} = \frac{1}{2m} \sum_{j=1}^{n} \hat{P}_j^2 + \frac{m}{2} \sum_{j=1}^{n} \mu_j \hat{Q}_j^2, \tag{42}$$

where the elements μ_j are the (positive) eigenvalues of A or D_A. The compatibility conditions (40) become

$$
\begin{aligned}
[\hat{H}, \hat{Q}_j] &= -\frac{i\hbar}{m} \hat{P}_j, \\
[\hat{H}, \hat{P}_j] &= i\hbar m \mu_j \hat{Q}_j.
\end{aligned}
\tag{43}
$$

It turns out that we will be able to find solutions for $\hat{Q}_j$ and $\hat{P}_j$ satisfying the CCs (43) and the Hamiltonian in equation (37) in terms of Lie superalgebra generators. The easiest way to establish such a result, is to introduce linear combinations of the unknown operators $\hat{Q}_j$ and $\hat{P}_j$ as follows:

$$b_j^\pm = \sqrt{\frac{m\sqrt{\mu_j}}{2\hbar}} \, \hat{Q}_j \mp \frac{i}{\sqrt{2\hbar m \sqrt{\mu_j}}} \, \hat{P}_j. \tag{44}$$

In terms of the operators $b_j^\pm$, which satisfy the adjointness relations $(b_j^\pm)^\dagger = b_j^\mp$, the Hamiltonian (37) can be rewritten as

$$\hat{H} = \sum_{j=1}^{n} \frac{\hbar\sqrt{\mu_j}}{2} \{b_j^+, b_j^-\} = \sum_{j=1}^{n} \frac{\hbar\sqrt{\mu_j}}{2} (b_j^+ b_j^- + b_j^- b_j^+). \tag{45}$$

The operators $b_j^\pm$ should not be confused with the boson operators $a_j^\pm$ of (14): the $b_j^\pm$ do *not* satisfy any particular commutation relations. Also in computing (45) one should be careful not to use relations that hold only in the canonical case. We can now express the compatibility conditions in terms of the newly introduced operators. These follow from (43) and are

$$\left[\hat{H}, b_j^\pm\right] = \pm \hbar \sqrt{\mu_j} \, b_j^\pm, \qquad (j = 1, 2, \ldots, n). \tag{46}$$

Thus we have:

Theorem 3 *The Wigner quantization of the system* (37) *has been reduced to the problem of finding $2n$ operators $b_j^\pm$ $(j = 1, \ldots, n)$ acting in a certain Hilbert space. These operators must satisfy $(b_j^\pm)^\dagger = b_j^\mp$ and*

$$\sum_{j=1}^n \sqrt{\mu_j} \, [\{b_j^+, b_j^-\}, b_k^\pm] = \pm 2 \sqrt{\mu_k} \, b_k^\pm, \qquad (k = 1, 2, \ldots, n). \qquad (47)$$

The Wigner quantization procedure is reversible, so that the knowledge of the operators $b_j^\pm$ allows us to reconstruct the observables $\hat{p}_r$ and $\hat{q}_r$. The Hamiltonian is given by equation (45).

The compatibility conditions (47) are triple relations, expressed by means of anti-commutators and commutators. In fact, (47) is equivalent to a quantum system describing an n-dimensional non-isotropic oscillator [21, Section 2]. For such systems, it is known that solutions in terms of Lie superalgebra generators exist [21]. Some specific solutions are related to the Lie superalgebras $\mathfrak{osp}(1|2n)$ and $\mathfrak{gl}(1|n)$, but not all solutions are known for $n > 1$.

Without going into the details of the further analysis, let us describe some properties of the $\mathfrak{gl}(1|n)$ solutions. First of all, one can verify that certain multiples of the odd basis elements of $\mathfrak{gl}(1|n)$ satisfy the relations (47) [21]. In this $\mathfrak{gl}(1|n)$ realization of the operators $b_j^\pm$, the Hamiltonian (45) becomes an element of the Cartan subalgebra. Next, one has to consider all unitary representations of $\mathfrak{gl}(1|n)$ (here, unitary refers to the fact that $(b_j^\pm)^\dagger = b_j^\mp$ should be satisfied in the $\mathfrak{gl}(1|n)$ representation). For certain sets of values of μ_j, these unitary representations are finite-dimensional (i.e. corresponding to the real form $\mathfrak{u}(1|n)$ of $\mathfrak{gl}(1|n)$). Then it is a matter of finding the weight structure of such a representation (e.g. by determining its character). Indeed, for any weight vector of weight $(k_0, k_1, \ldots, k_n)$, the corresponding $\hat{H}$ eigenvalue reads

$$\frac{\hbar}{n-1} (\sum_{j=1}^n \sqrt{\mu_j})(\sum_{j=0}^n k_j) - \sum_{j=1}^n \hbar k_j \sqrt{\mu_j} = \text{const} - \sum_{j=1}^n \hbar k_j \sqrt{\mu_j}, \qquad (48)$$

since $\sum_{j=0}^n k_j$ is constant for an irreducible representation of $\mathfrak{u}(1|n)$. Applying this, for example, to the Hamiltonian $\hat{H}_K$ (33) with Krawtchouk interaction, yields a spectrum of the form

$$\text{const} - \sum_{j=1}^n \hbar k_j \sqrt{\omega^2 - c(n - 2j + 1)/2}, \qquad (49)$$

where $(k_0, k_1, \ldots, k_n)$ runs over all weights of the representation under consideration, and the multiplicity is determined by the multiplicity of the weight. So the spectrum of $\hat{H}_K$ in Wigner's quantization looks formally very similar to that in canonical quantization, given by Proposition 2. There are however some important differences. First of all, in (36) the indices k_j run over all natural numbers, corresponding to all Fock space states. So the energy spectrum is

discrete but unbounded from above. Here, the indices assume only values corresponding to all weights of a certain finite-dimensional representation of $\mathfrak{u}(1|n)$. This implies that multiplicities of energy levels are in general quite different. More strikingly, a peculiar feature of Wigner quantization is that it allows finite-dimensional solutions, i.e. with a finite energy spectrum. Such solutions might be of relevance in a physical context. For more details about properties of the spectrum, and about relations to other Lie superalgebras, see [8].

4   Spin chain with a Krawtchouk interaction matrix

A final model where the new analytically solvable quantum Hamiltonians can be of use is related to quantum computation. In models of quantum computation, the transmission of a quantum state is an important aspect. S. Bose [22,23] introduced linear spin chains as a channel for short distance quantum communication. Transfer of data in such linear quantum registers has been the subject of many papers [22,24–26] (and references therein). An interesting situation arises if one assumes to have individual control of the nearest-neighbour interactions.

The transmission of quantum states can in principle be performed by a chain of qubits coupled via the Heisenberg or the XY interactions [27–30]. The idea of pre-engineered intercubit couplings has been discussed considerably [31,32]. One of the advantages of well-chosen controlled couplings is that one can obtain mirror inversion of a quantum state with respect to the center of the chain, and that perfect transfer of quantum states is possible [24,26,33].

Let us consider a by now classical system of $N + 1$ interacting qubits (spin $1/2$ particles) in a quantum register, with a Hamiltonian of XY type (for reasons of convenience, the index here runs from 0 to N):

$$\hat{H} = \frac{1}{2} \sum_{k=0}^{N-1} J_k(\sigma_k^x \cdot \sigma_{k+1}^x + \sigma_{k+1}^y \cdot \sigma_k^y) - \frac{1}{2} \sum_{k=0}^{N} h_k(\sigma_k^z - 1), \qquad (50)$$

where J_k is the coupling strength between the qubits located at sites k and $k+1$, and h_k is the "Zeeman" energy of a qubit at site k. So the subindex k ($k = 0, 1, 2, \ldots, N$) labels the position of the qubit in the chain, and the superindex refers to the Pauli matrices σ^x, σ^y and σ^z.

To describe the Hilbert space associated with the Hamiltonian, one adopts a standard fermionization technique [34]. Then the Jordan-Wigner transformation [35] allows to rewrite the Hamiltonian (50) in terms of fermion operators f_k and $f_k^\dagger$ ($k = 0, 1, \ldots, N$):

$$\hat{H} = \sum_{k=0}^{N-1} J_k(f_k^\dagger f_{k+1} + f_{k+1}^\dagger f_k) + \sum_{k=0}^{N} h_k f_k^\dagger f_k. \qquad (51)$$

This Hamiltonian can be interpreted as describing a set of $N + 1$ fermions on a chain with nearest-neighbour interaction (hopping between adjacent sites of the chain), and subject to a non-uniform magnetic field denoted by h_k ($k = 0, 1, \ldots, N$). We shall assume that the system is initially in its ground state

$|\mathbf{0}\rangle = |00\cdots 0\rangle = |0\rangle \otimes |0\rangle \otimes \cdots \otimes |0\rangle$, where $|0\rangle$ denotes the spin down state. Let $|k\rangle = |00\cdots 010\cdots 0\rangle = f_k^\dagger |\mathbf{0}\rangle$ $(k = 0, 1, \ldots, N)$ denote a state in which there is a single fermion at the site k and all other sites are empty, i.e. $|k\rangle$ describes the state in which the spin at the site k has been flipped to $|1\rangle$. Clearly, the set of states $|k\rangle$ $(k = 0, 1, \ldots, N)$ forms a basis for the single-fermion states of the system, and we can represent these by the standard unit vectors in column matrix form:

$$|k\rangle = \begin{pmatrix} 0 \\ 0 \\ \vdots \\ 1 \\ \vdots \\ 0 \end{pmatrix} \qquad (k = 0, 1, \ldots, N). \tag{52}$$

In this single-fermion basis, the Hamiltonian $\hat{H}$ takes the matrix form

$$M = \begin{pmatrix} h_0 & J_0 & 0 & \cdots & & 0 \\ J_0 & h_1 & J_1 & \cdots & & 0 \\ 0 & J_1 & h_2 & \ddots & & \\ \vdots & \vdots & \ddots & \ddots & & J_{n-1} \\ 0 & 0 & & & J_{N-1} & h_n \end{pmatrix}. \tag{53}$$

The dynamics (time evolution) of the system is completely determined by the eigenvalues ϵ_j and eigenvectors ϕ_j of this matrix. It is then a standard technique [33, 34] to describe the n-fermion eigenstates of $\hat{H}$ $(n \leq N)$ using the single-fermion eigenstates ϕ_j and Slater determinants. For this reason we concentrate here on the single-fermion eigenstates.

Once we have arrived at the matrix (53), one recognizes a tridiagonal interaction matrix and the methods of Section 2 can be applied. In particular, one can perform the spectral decomposition (6) with an orthogonal matrix U, and $D = \mathrm{diag}(\epsilon_0, \epsilon_1, \ldots, \epsilon_N)$. The entries of D are the single-fermion energy eigenvalues, and the columns of the matrix U are the (orthonormal) eigenvectors of M, i.e. the single-fermion eigenstates:

$$\phi_j = \begin{pmatrix} U_{0j} \\ U_{1j} \\ \vdots \\ U_{Nj} \end{pmatrix} = \sum_{k=0}^{N} U_{kj} |k\rangle = \sum_{k=0}^{N} U_{kj} f_k^\dagger |\mathbf{0}\rangle \qquad (j = 0, 1, \ldots, N), \tag{54}$$

with $\hat{H}\phi_j = M\phi_j = \epsilon_j \phi_j$. From the orthogonality of U, the inverse relation follows:

$$|k\rangle = \sum_{j=0}^{N} U_{kj} \phi_j. \tag{55}$$

We now turn to the dynamics of the system under consideration, described by the time evolution operator $\exp(-it\hat{H})$. Assume that the "state sender" is located at site s of the spin chain, and the "state receiver" at site r (s and r are site labels, belonging to $\{0, 1, \ldots, N\}$). At time $t = 0$ the sender turns the system into the single spin state $|s\rangle$. After a certain time t, the system is in the (mixed) state $\exp(-it\hat{H})|s\rangle$. So the transition amplitude of an excitation from site s to site r of the spin chain is given by the modulus of

$$F_{r,s}(t) = (r|\exp(-it\hat{H})|s). \tag{56}$$

This is one of the central quantities to be computed in this context. Note that it can be expressed by means of the orthogonal matrix U appearing in (6). Indeed, using the expansion (55) and orthogonality of the states ϕ_j, one finds:

$$F_{r,s}(t) = (r|\exp(-it\hat{H})|s) = \langle \sum_{k=0}^{N} U_{rk}\phi_k | \exp(-it\hat{H}) \sum_{j=0}^{N} U_{sj}\phi_j \rangle$$

$$= \langle \sum_{k=0}^{N} U_{rk}\phi_k | \sum_{j=0}^{N} U_{sj} e^{-it\epsilon_j} \phi_j \rangle$$

$$= \sum_{j=0}^{N} U_{rj} U_{sj} e^{-it\epsilon_j}. \tag{57}$$

The purpose of this section is to show that various interesting closed form expressions can be given for this crucial quantity $F_{r,s}(t)$, in the case that the fixed values characterizing the system (the values J_k and h_k) are related to the Jacobi matrix of a set of discrete orthogonal polynomials, just as this was the case in Section 2. Again, we shall illustrate this by means of the example of Krawtchouk polynomials. Let us therefore identify the matrix (53) with the Jacobi matrix (28) of the Krawtchouk polynomials (note that the replacement of J_k by $-J_k$ does not lead to essential changes in the formulation, as it would only give rise to sign factors $(-1)^{j+k}$ in the matrix elements U_{jk} and $(-1)^{r+s}$ in the amplitudes $F_{r,s}(t)$). Under this identification, the matrix elements of U are (normalized) Krawtchouk polynomials, see eq. (30), and the corresponding energy eigenvalues are $\epsilon_j = j$ ($j = 0, 1, \ldots, N$).

This implies that we can determine the transition amplitude as follows:

$$F_{r,s}(t) = \sum_{k=0}^{N} U_{rk} U_{sk} e^{-it\epsilon_k} = \sum_{k=0}^{N} \tilde{K}_r(k) \tilde{K}_s(k) e^{-itk}$$

$$= \frac{1}{\sqrt{d_r d_s}} \sum_{k=0}^{N} w(k) K_r(k) K_s(k) e^{-itk}. \tag{58}$$

So we need to compute the quantity in (58). First of all, note that in general $F_{r,s}(t)$ is a periodic function of t. In particular, it follows from (58) and the orthogonality relation (23) that $F_{r,s}(t) = \delta_{rs}$ for $t = 0$ and for any multiple of

2π. So after a time span of 2π, the system is back in its original state where only the spin at the sending site s is flipped.

The purpose is now to compute (58) explicitly. Rewriting the polynomials in (58) as ${}_2F_1$-series, this sum reduces to a classical summation formula given for example in [36, p. 84, (8)]. This leads immediately to the following closed form expression:

$$F_{r,s}(t) = \sqrt{\binom{N}{r}\binom{N}{s}}(\sqrt{p(1-p)})^{r+s}(1 - e^{-it})^{r+s}(1 - p + pe^{-it})^{N-r-s}$$

$$\times \ {}_2F_1\left(\begin{matrix}-r,-s\\-N\end{matrix};\frac{-e^{-it}}{p(1-p)(1-e^{-it})^2}\right). \tag{59}$$

Some special cases of this general formula are worth discussing.

Let us consider the case when the sender is located at site 0, i.e. $s = 0$. Then (59) yields

$$F_{r,0}(t) = \sqrt{\binom{N}{r}}(\sqrt{p(1-p)})^r(1 - e^{-it})^r(1 - p + pe^{-it})^{N-r}. \tag{60}$$

So far, p $(0 < p < 1)$ is still a free parameter. A special case occurs when $p = 1/2$:

$$F_{r,0}(t) = \frac{1}{2^N}\sqrt{\binom{N}{r}}(1 - e^{-it})^r(1 + e^{-it})^{N-r}, \qquad (p = 1/2) \tag{61}$$

giving

$$|F_{r,0}(t)| = \sqrt{\binom{N}{r}}\left|\sin\left(\frac{t}{2}\right)\right|^r\left|\cos\left(\frac{t}{2}\right)\right|^{N-r}. \qquad (p = 1/2) \tag{62}$$

In other words,

$$F_{r,0}(\pi) = \delta_{r,N}. \qquad (p = 1/2) \tag{63}$$

This is the situation of "perfect state transfer" described already in [33]: at time $t = \pi$ the system is in the state with all spins down except at site N the spin is up. So for this time there is perfect state transfer from site 0 to site N.

More generally, let us specialize the expression (59) for time $t = \pi$:

$$F_{r,s}(\pi) = \sqrt{\binom{N}{r}\binom{N}{s}}(\sqrt{4p(1-p)})^{r+s}(1 - 2p)^{N-r-s}$$

$$\times \ {}_2F_1\left(\begin{matrix}-r,-s\\-N\end{matrix};\frac{1}{4p(1-p)}\right). \tag{64}$$

This expression shows once again that taking the free parameter $p = 1/2$ yields a special case:

$$F_{r,s}(\pi) = \delta_{r+s,N}. \qquad (p = 1/2) \tag{65}$$

So for $p = 1/2$ there is also perfect state transfer between the sites s and $N - s$.

We have shown here how a spin chain (51) with interaction matrix (53) determined by a Jacobi matrix related to discrete orthogonal polynomials gives rise to an analytic solution of transition amplitudes in terms of these orthogonal polynomials. Only the simplest case of Krawtchouk polynomials has been discussed here; more detailed work with other families of orthogonal polynomials is in preparation [37].

5 Conclusions

Quantum Hamiltonians characterized by a tridiagonal interaction matrix play an interesting role in various models. When this tridiagonal interaction matrix coincides with the Jacobi matrix of a system of discrete orthogonal polynomials, many quantities related to the model can be computed explicitly. In the model of harmonic oscillators with some nearest-neighbour interaction, the spectrum of the Hamiltonian is determined in closed form (or the Hamiltonian is analytically solvable), as it is related to factors appearing in the three term recurrence relation for the orthogonal polynomials. In the model of a spin chain with a nearest-neighbour hopping term, one obtains explicit formulas for transition amplitudes, as in this case there is a relation with some bilinear generating function of the orthogonal polynomials.

In this paper, we have illustrated these aspects by means of some examples, and indicated how to approach this in general. We have also treated an alternative quantization of the first model of interaction harmonic oscillators, namely Wigner quantization. In that case, representations of Lie superalgebras appear in the solutions.

Acknowledgments

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