Quantum chaos as delocalization in Krylov space

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(Received 21 January 2020; revised 31 May 2020; accepted 23 July 2020; published 19 August 2020)

We analyze local operator growth in nonintegrable quantum many-body systems. A recently introduced universal operator growth hypothesis proposes that the maximal growth of Lanczos coefficients in the continued fraction expansion of the Green's function reflects chaos of the underlying system. We first show that the continued fraction expansion, and the recursion method in general, should be understood in the context of a completely integrable classical dynamics in Krylov space. In particular, the time-correlation function of a physical observable analytically continued to imaginary time is a tau-function of integrable Toda hierarchy. We use this relation to generalize the universal operator growth hypothesis to include arbitrarily ordered correlation functions. We then proceed to analyze the singularity of the time-correlation function, which is an equivalent sign of chaos to the maximal growth of Lanczos coefficients, and we show that it is due to delocalization in Krylov space. We illustrate the general relation between chaos and delocalization using an explicit example of the Sachdev-Ye-Kietaev model.

DOI: 10.1103/PhysRevB.102.085137

Introduction. The time-correlation function of local operators is one of the standard probes of quantum many-body physics. It characterizes a system's linear response and transport. With the exception of a few integrable models, the explicit form of the time-correlation function is not known, and a variety of methods have been devised to describe its behavior in different limits. Among them is the recursion method [1–3], briefly described below, which is commonly used for analytic and numerical approximations. In this paper, we show that the recursion method should be understood as a part of a more general construction, defining completely integrable dynamics in Krylov space. In particular, in full generality, the time-correlation function of a physical observable, analytically continued to Euclidean (imaginary) time, is a tau-function of the integrable Toda chain. Previously known examples [4–7] in which a quantum correlation function was related to a classical tau-function of an integrable hierarchy were in the context of very particular integrable or supersymmetric theories. Here we consider generic dynamical systems and generic observables.

One of the open questions of quantum many-body dynamics is how to characterize chaotic behavior. This question connects very different pursuits from quantum gravity [8] to mesoscopic thermodynamics [9]. Recently it was proposed [10] that the time-correlation function of local operators reflects underlying quantum chaotic behavior through the maximal growth of Lanczos coefficients (introduced below); see also [11–13] for related work. The maximal growth of Lanczos coefficients can be reformulated as singularity of the time-correlation function in imaginary time [14]. We apply the relation to the Toda chain to elucidate this picture and show that the singularity in imaginary time is due to delocalization of the operator in Krylov space.

Recursion method and Krylov space. We begin by reminding the reader about the basics of the recursion method [15,16], which includes Krylov space construction and Lanczos coefficient expansion. The starting point is the time-correlation function of some operator A,

$$C(t) = \langle A(t), A\rangle, \tag{1}$$

defined with help of a Hermitian bilinear form in the space of operators,

$$\langle A, B\rangle \equiv \mathrm{Tr}(A^\dagger \rho_1 B \rho_2) = \langle B, A\rangle^*. \tag{2}$$

Here ρ_1, ρ_2 are some Hermitian positive-semidefinite operators that commute with the Hamiltonian H. Therefore, the adjoint action $[H,\ ]$ is self-adjoint with respect to $\langle\ ,\ \rangle$. Colloquially, (2) is a scalar product in the space of operators, with the caveat that it might be positive-semidefinite rather than definite. For any initial $A_0 = A$, one can define Krylov space, which is the space of linear combinations of all operators of the form $[H, [H, [\dots, A]]]$. Alternatively, Krylov space is the minimal subspace in the space of all operators, which includes time-evolved $A(t)$ for any t. Next, we define a basis in the Krylov space A_k via the iterative relation

$$A_{n+1} = [H, A_n] - a_n A_n - b_{n-1}^2 A_{n-1}, \tag{3}$$

and we require A_k to be mutually orthogonal, $\langle A_k, A_l\rangle = 0$ for $k \neq l$. Orthogonality of A_k fixes coefficients a_n, b_n to be

$$a_n = \frac{\langle [H, A_n], A_n\rangle}{\langle A_n, A_n\rangle}, \quad b_n^2 = \frac{\langle A_{n+1}, A_{n+1}\rangle}{\langle A_n, A_n\rangle},\ n \geqslant 0. \tag{4}$$

Coefficients a_n, b_n are called Lanczos coefficients. They appear in the continued fraction expansion of the Green's function associated with $C(t)$. While this is not important for our discussion, this is one of the central relations of the recursion method [1–3], and we explain it in the Appendix.

For any Hermitian operator, its norm defined with the help of (2) is manifestly real and non-negative. It is therefore convenient to introduce $q_n = \ln\langle A_n, A_n\rangle$ such that

$$G_{nm} = \langle A_n, A_m\rangle = \delta_{nm} e^{q_n}. \tag{5}$$

In (3) we formally require $b_{-1} = 0$.

In what follows, we focus on the Euclidean time evolution,

$$O(t) \equiv e^{tH} O e^{-tH}, \tag{6}$$

where t is Euclidean (imaginary) time. An operator evolved in conventional (Minkowski) time is $O(-it)$. With the help of (3), adjoin action of H in the Krylov basis A_n can be represented by a Jacobi (i.e., tridiagonal) matrix L,

$$[H, A_n] = \sum_m L_{nm} A_m, \quad L = gMg^{-1}, \tag{7}$$

$$g = \mathrm{diag}(e^{q_0/2}, e^{q_1/2}, \dots), \tag{8}$$

$$M = \begin{pmatrix} a_0 & b_0 & 0 & \ddots \\ b_0 & a_1 & b_1 & \ddots \\ 0 & b_1 & a_2 & \ddots \\ \ddots & \ddots & \ddots & \ddots \end{pmatrix}. \tag{9}$$

Matrix L is usually called the Liouvillian because it generates time evolution of an operator expanded in the Krylov basis A_n. The tridiagonal form of L and M allows for simple numerical evaluation of e^{iMt}, i.e., time evolution in the Krylov basis. This underlines the use of the Krylov space method (also known as the Lanczos method) in numerical applications.

Toda chain flow in Krylov space. At this point we would like to establish a connection between the recursion method and classical integrable dynamics. As a generalization of (5), we define

$$G_{nm}(t) = \langle A_n(t), A_m\rangle \tag{10}$$

and evaluate it in terms of Lanczos coefficients (we use matrix notations here for brevity),

$$G(t) = g\, e^{Mt} g^T. \tag{11}$$

The original correlation function is then $C(t) = G_{00}(t) = \langle A_0, A_0\rangle (e^{Mt})_{00}$.

We leave $G(t)$ aside for a moment and show that Lanczos coefficients a_n, b_n can naturally be promoted to be t-dependent functions. Later we will show that they satisfy Toda chain equations of motion [17]. First, we interpret $\langle A(t), B\rangle$ for two arbitrary operators A, B as a t-dependent family of scalar products (Hermitian bilinear forms),

$$\langle A, B\rangle_t \equiv \langle A(t), B\rangle. \tag{12}$$

It is easy to see that $\langle\ ,\ \rangle_t$ can be defined with the help of (2) with some new t-dependent $\rho^t_{1,2}$,

$$\rho^t_1 = e^{tH/2} \rho_1\, e^{tH/2}, \quad \rho^t_2 = e^{-tH/2} \rho_2\, e^{-tH/2}. \tag{13}$$

For any real t, $\rho^t_{1,2}$ satisfy the requirements we outlined for $\rho_{1,2}$ above: they are Hermitian positive-semidefinite and commute with H. We therefore can apply the recursion method to define the Krylov basis starting from the same initial A for any given value of t. This defines the family of orthogonal bases $A^t_n, A^t_0 \equiv A$,

$$G^t_{nm} \equiv \langle A^t_n, A^t_m\rangle_t = \delta_{nm} e^{q_n(t)}, \tag{14}$$

where a_n, b_n, and q_n are now t-dependent,

$$a_n(t) = \frac{\langle [H, A^t_n], A^t_n\rangle_t}{\langle A^t_n, A^t_n\rangle_t}, \tag{15}$$

$$b^2_n(t) = e^{q_{n+1}-q_n}, \quad q_n(t) = \ln\langle A^t_n, A^t_n\rangle_t. \tag{16}$$

With the help of $a_n(t), b_n(t), q_n(t)$ we also define t-dependent matrices $M(t)$ and $g(t)$; see Eqs. (8) and (9).

A crucial observation is that $G_{nm}(t)$ (10) and G^t_{nm} (14) are the matrix representation of the same scalar product $\langle\ ,\ \rangle_t$ written in terms of two different bases, A_n and A^t_n. They are therefore related by a change of coordinates,

$$G(t) = z(t) G^t z(t)^T, \tag{17}$$

$$A_n = \sum_m z_{nm}(t) A^t_m. \tag{18}$$

Going back to the definition (3), for any given t, basis element A^t_n is a linear combination of nested commutators $\underbrace{[H, \dots, [H, A]]}_{k\ \text{times}}$ with $0 \leqslant k \leqslant n$ such that the coefficient in front of the nested commutator of degree n is exactly 1. Therefore, matrix $z(t)$, which transforms basis A^t_n into basis $A_n \equiv A^{t=0}_n$, is lower-triangular with the identities on the diagonal. For convenience we rewrite (17) using (11) and express G^t in terms of $g(t)$,

$$G(t) = g(0) e^{M(0)t} g(0)^T = z(t) g(t) g(t)^T z(t)^T. \tag{19}$$

The right-hand side of (19) defines the so-called orispherical coordinate system (q_n, z_{nm}), $n > m$, on the space of symmetric positive-definite matrices G. The explicit time dependence of $G(t)$ given by (19) provides that

$$\frac{d}{dt}(G^{-1}\dot{G}) = 0. \tag{20}$$

Thus, $G(t)$ describes a geodesic flow on the space of symmetric positive-definite matrices, which is projected onto the space of diagonal matrices (parametrized by coordinates q_n) by the group of lower-triangular matrices with the identities on the diagonal. This geodesic flow is described by an open Toda chain, which can be shown by applying the Hamiltonian reduction formalism toward the original geodesic flow; see [18]. From here it follows that $q_n(t)$ defined via (16) satisfies the following set of equations:

$$\ddot{q}_n = e^{q_{n+1}-q_n} - e^{q_n - q_{n-1}}, \tag{21}$$

which are the equations of motion of a completely integrable Toda chain [17]. This is the main result of the first part of the paper.

There are several useful ways to rewrite Eq. (21). First, using the trivial redefinition

$$a_n(t) \equiv \dot{q}_n, \quad b_n(t) \equiv e^{(q_{n+1}-q_n)/2}, \tag{22}$$

we can express Toda chain equations of motion (21) in the so-called Flaschka form [19]

$$\dot{a}_n = b_n^2 - b_{n-1}^2, \quad \dot{b}_n = b_n(a_{n+1} - a_n)/2. \tag{23}$$

Note that (22) is consistent with (15) if we take into account that the derivative of A_n^t with respect to t is a linear combination of A_k^t for $0 \leqslant k < n$. Alternatively, Toda equations can be straightforwardly rewritten in the so-called Hirota's bilinear form [20],

$$\tau_n \ddot{\tau}_n - \dot{\tau_n}^2 = \tau_{n+1}\tau_{n-1}, \quad \tau_{-1} \equiv 1, \tag{24}$$

where $\tau_n = \exp(\sum_{0\leqslant k\leqslant n} q_n)$. In particular,

$$\tau_0(t) = e^{q_0(t)} = C(t), \tag{25}$$

which establishes in full generality that the time-correlation function analytically continued to Euclidean time is a tau-function of Toda hierarchy.

At this point we would like to make a number of remarks outlining the role of completely integrable classical dynamics in the context of the recursion method. By virtue of the identity $\langle A(t/2), B(t/2)\rangle = \langle A, B\rangle_t$ for any A and B, operators $A_n^t(t/2)$ define the orthogonal Krylov basis associated with the scalar product $\langle\ ,\ \rangle$ and the initial operator $A_0 = A(t/2)$. Corresponding Lanczos coefficients are $a_n(t)$ and $b_n(t)$. This follows from the fact that the relation (3) is linear, and hence it will hold if all operators are evolved in time. Thus, the flow described by the Toda chain can be defined solely in terms of the original scalar product $\langle\ ,\ \rangle$ by considering different initial vectors of the Krylov basis. Furthermore, since $e^{-q_n(0)/2}A_n$ and $e^{-q_n(t)/2}A_n^t(t/2)$ are orthonormal bases for the same scalar product, they must be related by some orthogonal transformation Q^T,

$$\sum_m Q_{nm}^T(t/2)e^{-q_m(0)/2}A_m = e^{-q_n(t)/2}A_n^t(t/2). \tag{26}$$

Evolving this equation in time by $-t/2$ and using the relation (18) between A_n and A_n^t, we find

$$e^{M(0)t} = Q(t)R(t), \quad R^T(t/2) = g(0)^{-1}z(t)g(t). \tag{27}$$

This defines QR decomposition of $e^{M(0)t}$, i.e., representation as a product of an orthogonal matrix Q and lower-triangular matrix R. Any real-valued matrix admits QR decomposition, but it plays an important role in the context of the Toda chain [21], and in our analysis below.

We did not require the Hermitian form $\langle\ ,\ \rangle$ to be positive-definite, merely positive-semidefinite. Therefore, the coefficient b_n^2 given by (4) may vanish either because A_{n+1} vanishes as an operator, or because it has zero "norm" $\langle A_{n+1}, A_{n+1}\rangle = 0$. In either case, time-evolved $A(t)$ will be a linear combination of only the first n basis elements A_k, and therefore $C(t)$ will be described in terms of a finite Toda chain. Matrix G_{kl} in this case will be defined for $0 \leqslant k, l \leqslant n$ and will be finite positive-definite. Thus, without loss of generality, matrix G is always positive-definite, which justifies taking the inverse in (20). This completes the construction of the recursion method as a part of the Toda chain flow in Krylov space.

This result is very general. The construction above is linear in the scalar product, and therefore applies to any linear combination of (2), i.e., when

$$\langle A, B\rangle \equiv \sum_i \mathrm{Tr}\big\langle A^\dagger \rho_1^{(i)} B \rho_2^{(i)}\big\rangle. \tag{28}$$

This may appear, e.g., in the context of differently ordered thermal correlators. For example, if $\rho_1 = \rho_2 = \rho^{1/2}$, $\rho = e^{-\beta H}/Z$, this defines symmetric ordering with $a_n = 0$. A conventional thermal correlator is obtained by $\rho_1 = \mathcal{I}$, $\rho_2 = \rho$. We have show that Lanczos coefficients for these two cases are related to each other via time evolution of Toda equations of motion from $t = 0$ to $t = \beta/2$.

Quantum chaos and delocalization. The relation to the Toda chain provides a way to analyze the time-correlation function. Below we apply it to elucidate chaos in quantum many-body systems. The growth of $C(t)$ in Euclidean time is qualitatively different in integrable (solvable) and generic lattice systems [14]. Considering the thermodynamic limit in known integrable examples, $C(t)$ is an entire function of a complex parameter t. On the contrary, an accurate counting of nested commutators appearing in the Taylor series expansion of $C(t)$ suggests that in general, i.e., the nonintegrable case, $C(t)$ will be singular at some finite $t = t^*$. This behavior is confirmed by an explicit example of [22]. The same singular behavior for the chaotic models follows from the conjecture of [10], which associates chaos with the maximal rate of growth of Lanczos coefficients permitted by analyticity of $C(t)$ at $t = 0$, $b_n \propto n$. An equivalent formulation in terms of the power spectrum of $C(t)$ was advocated earlier in [23].

The original analysis of [10] assumed $a_n = 0$. The Toda chain formalism provides an easy way to extend this result. From the equations of motion (23) it follow that linear growth $b_n \propto n$ is consistent with at most linear growth of a_n, and the slope of a_n cannot exceed twice the slope of b_n. This can be illustrated with the help of a family of exact solutions. Combining (23) into

$$\frac{d^2}{dt^2}\ln b_n^2 = b_{n+1}^2 - 2b_n + b_{n-1}^2, \tag{29}$$

and assuming $b_n^2 = b^2(t)p(n)$, where $p(n)$ is an arbitrary quadratic polynomial, we find

$$a_n(t) = (2n + c)J\cot(J(t_0 - t)), \tag{30}$$

$$b_n^2(t) = \frac{(n+c)(n+1)J^2}{\sin^2(J(t_0 - t))}. \tag{31}$$

This family is associated with the tau-function $\tau_0 \propto [\sin(J(t_0 - t))]^{-c}$, which is the time-correlation function of the Sachdev-Ye-Kitaev model [10,24]. The same solution with $c = 2$ in the $J \to 0$ limit also appeared in [25] in the context of $\mathcal{N} = 2$ SYM. At large n, $a_n/b_n \propto 2\sin(J(t_0 - t))$. Thus, in general, chaotic behavior is reflected by the linear growth of both a_n and b_n, parametrized by J and dimensionless $|\gamma| \leqslant 1$,

$$\lim_n \left(b_n^2 - a_n^2/4\right)/n^2 = J^2, \quad \lim_n a_n/b_n = 2\gamma. \tag{32}$$

The asymptotic behavior of a_n, b_n controls the location of the singularity of $C(t)$ at $t^* = \arcsin(\gamma)/J$.

Singular behavior of the time-correlation function can be further elucidated. As a starting point, we assume that $C(t) = G_{00}(t)$ is a smooth function, together with its derivatives for

$0 \leqslant t < t^*$, and it diverges at $t = t^*$. From here it follows that for $n, m \geqslant 0$, $G_{nm}(t)$ defined in (10) is regular for $0 \leqslant t < t^*$. Indeed, different matrix elements $G_{nm}(t)$ are related by the differential operator

$$G_{n+1,m} = \left(\frac{d}{dt} - a_n\right) G_{nm} - b_{n-1}^2 G_{n-1,m}. \tag{33}$$

Therefore, all G_{nm} are regular for $0 \leqslant t < t^*$, provided $C(t)$ is sufficiently smooth.

Using QR decomposition (27), we can decompose

$$R_{00}(t/2)^2 = C(t)/C(0), \tag{34}$$

and we conclude that $R_{00}(t)$ is regular for $0 \leqslant t < t^*/2$ and diverges at $t = t^*/2$. Using (27) again we can decompose $A(t)$ into an orthonormal Krylov basis,

$$e^{-q_0(0)/2} A(t) = \sum_n c_n(t) (e^{-q_n(0)/2} A_n), \tag{35}$$

where

$$c_n(t) \equiv e^{-[q_0(0)+q_n(0)]/2} G_{0n}(t) = R_{00}(t) Q_{n0}(t). \tag{36}$$

Here $R_{00}(t)$ is the norm of the operator, and the unit vector $Q_{n0}(t)$ specifies projection on a particular basis element. Regularity of $G_{0n}(t)$ at $t = t^*/2$ and divergence of $R_{00}(t)$ at $t = t^*/2$ implies that $Q_{n0}(t^*/2)$ for all n has to vanish. This is a manifestation of delocalization in Krylov space: at $t = t^*/2$ the operator $A(t)$ spreads across the whole Krylov space, such that its norm diverges, while its projection on any particular normalized basis element is finite. The same can be seen from the inverse participation ratio I,

$$I \equiv \left(\sum_n Q_{n0}^4\right)^{-1}, \tag{37}$$

which diverges at $t = t^*/2$. This can be seen directly from the explicit solutions (30). We show in the Appendix that the solutions correctly capture universal behavior near $t = t^*/2$.

Finally, we would like to contrast the behavior of $A(t)$ in Krylov space and the singularity of I near $t = t^*/2$ for (30) with the behavior for integrable models. Starting from $b_n^2 = b^2 p(n)$, where $p(n)$ is a linear function, one finds an explicit solution illustrating "integrable" behavior $b_n \propto n^{1/2}$. The corresponding tau-function grows double-exponentially, $\tau_0 \propto \exp\{e^{m(t-t_0)}\}$, which is the behavior of $C(t)$ in generic one-dimensional systems [14]. This further emphasizes that nonintegrable one-dimensional systems cannot be considered fully chaotic. In the limit $m \to 0$, the tau-function becomes Gaussian, $\tau_0 \propto e^{a(t-t_0)^2/2}$. In both cases, $A(t)$ is moving as a localized wave packet in Krylov space, with the inverse participation ratio growing with time exponentially when $m \neq 0$ or merely linearly when τ_0 is a Gaussian. Technical details can be found in the Appendix.

Discussion. In this paper, we established explicit representation for the Euclidean time evolution of the time-correlation function as a classical dynamics of the integrable Toda chain. We have subsequently used the Toda chain formalism to elucidate the behavior of the time-correlation function in nonintegrable quantum many-body systems. We have extended the conjecture of [10] to include nonvanishing a_n. We have also demonstrated that singularity along the imaginary time axis, which is a generic behavior for nonintegrable systems, is due to delocalization in Krylov space.

The obtained connection between the recursion method and the Toda chain is likely to lead to new practical improvements in the numerical applications, as suggested by many other uses of the Toda chain in the context of computational algorithms [26].

Tau-functions of completely integrable systems have free-fermion representation [27]. It is a natural question to ask how this representation may appear in the context of the time-correlation function of a *generic* Hamiltonian system. The construction presented in this paper does not require the system to be quantum. In the classical case, scalar product (2) can be defined as an integral over the phase space, and the adjoint action $[H, \ ]$ in (3) will be substituted by the Poisson brackets. Further, an arbitrary classical system can be reformulated in terms of a supersymmetric path integral, which includes auxiliary fermionic degrees of freedom [28]. We expect the free-fermion representation to follow from there.

One of our main results is the relation between nonintegrability of the original physical system and delocalization in Krylov space. This result can be understood in the context of a general idea that localization versus ergodicity in physical space corresponds to delocalization in the auxiliary "Fock space" of a "particle" moving on a graph [29]. This idea has been further developed in the context of many-body localization in [30]. In a general case, construction of the appropriate graph is not clear. Our study suggests that the Krylov basis provides a representation of the "Fock space," with the tridiagonal Liouvillian matrix M describing hoping of a particle on a one-dimensional graph.

Acknowledgments. We thank A. Avdoshkin, B. Fine, and Z. Komargodski for discussions. A.D. acknowledges support of the Russian Science Foundation (Project No. 17-12-01587). The work of A.G. was supported by a Basis Foundation fellowship and RFBR Grant No. 19-02-00214. The authors thank the Simons Center for Geometry and Physics at State University of New York, Stony Brook, where some of this research was performed, for the hospitality and support.

APPENDIX

1. Toda miscellanea

Here we mention certain standard results about the Toda chain that are used in the other parts of the paper.

a. Toda EOM in Lax form

In (26) we introduce an orthogonal matrix Q that maps between the family of orthonormal bases $A_n^t(t/2)e^{-q_n(t)/2}$, parametrized by t, all being associated with the same scalar product $\langle \ , \ \rangle$. Matrix $M(t)$ is simply the matrix of the adjoint action $[H, \ ]$ written in the t-basis. From here it follows that the t-dependence of $M(t)$ is an isospectral deformation,

$$M(t) = Q^T(t/2) M(0) Q(t/2). \tag{A1}$$

Written in differential form, this becomes the Toda equation of motion written in Lax form [21],

$$\dot{M}(t) = [B(t), M(t)], \quad \dot{Q}^T(t) = 2B(2t)Q^T(t), \tag{A2}$$

$$B = \frac{1}{2}\begin{pmatrix} 0 & b_0 & 0 & \ddots \\ -b_0 & 0 & b_1 & \ddots \\ 0 & -b_1 & 0 & \ddots \\ \ddots & \ddots & \ddots & \ddots \end{pmatrix}. \tag{A3}$$

b. Hankel determinant representation

Tau-functions of Toda hierarchy $\tau_n = \exp(\sum_{0\leqslant k\leqslant n} q_n)$ are the leading principal minors of matrix $G_{nm}(t)$, as follows from Eq. (19), the lower-triangular form of z and $z_{nn} = 1$. They can also be expressed concisely in terms of $C(t) = e^{q_0(t)}$ and its derivatives. Namely, we introduce $(n+1)\times(n+1)$, $n \geqslant 0$, the matrix

$$\mathcal{M}^{(n)}_{ij} = C^{(i+j)}(t), \tag{A4}$$

where $C^{(k)}(t)$ stands for the kth derivative of C. Then

$$\tau_n = \det \mathcal{M}^{(n)}. \tag{A5}$$

2. Continued fraction representation

Continued fraction representation of the Green's function,

$$\mathrm{G}(z) = \int_0^\infty e^{-zt}\, C(t)\, dt, \tag{A6}$$

is the central part of the recursion method. From the definition above and representation (11), we readily find

$$\mathrm{G}(z) = \left(\frac{1}{z\mathcal{I} - M}\right)_{00}, \tag{A7}$$

provided the original operator is normalized, $C(0) = 0$. When matrix M is infinite, the inverse matrix $(z\mathcal{I} - M)^{-1}$ should be understood in the formal sense. It is convenient to consider M to be finite, such that a_n are defined for $0 \leqslant n \leqslant N+1$ and b_n for $0 \leqslant n \leqslant N$. Then we introduce $M^{(n)}$ as the $(N-n)\times(N-n)$ bottom-right corner submatrix of M. By Δ_n we denote a characteristic polynomial of $M^{(n)}$,

$$\Delta_n = \det(z\mathcal{I} - M^{(n)}). \tag{A8}$$

Then $\mathrm{G}(z) = \Delta_1/\Delta_0$.

To obtain the continued fraction representation, we notice that Δ_n satisfies the following iterative relation:

$$\Delta_n = (z - a_n)\Delta_{n+1} - b_n^2\,\Delta_{n+2}. \tag{A9}$$

If one defines $s_n = \Delta_n/\Delta_{n+1}$, then

$$s_n = (z - a_n) - b_n^2/s_{n+1}. \tag{A10}$$

From here it follows that

$$\mathrm{G}(z) \equiv \frac{1}{s_0} = \frac{1}{z - a_0 - \frac{b_0^2}{s_1}} = \frac{1}{z - a_0 - \frac{b_0^2}{z - a_1 - \frac{b_1^2}{s_2}}} = \cdots .$$

Continued fraction representation plays an important role in the context of the Toda chain as well. In this case, $\mathrm{G}(z,t)$ is defined by (A7) with the t-dependent $M(t)$. Using (19) we readily find

$$\frac{C(t+s)}{C(t)} = (e^{sM(t)})_{00}, \tag{A11}$$

and therefore

$$\mathrm{G}(z,t) = \frac{\int_t^\infty C(t')e^{-zt'}dt'}{C(t)}. \tag{A12}$$

Green's function $\mathrm{G}(z,t)$ can be written in terms of the eigenvalues λ_i of M and non-negative r_n, $\sum_n r_n^2 = 1$,

$$\mathrm{G}(z,t) = \frac{\sum_n \frac{r_n^2}{z-\lambda_n}}{\sum_n r_n^2}. \tag{A13}$$

Then the time dependence of G is described by the gradient flow [31],

$$\frac{d\lambda_k}{dt} = 0, \quad \frac{dr_k}{dt} = -\frac{\partial V}{\partial r_k}, \quad V = \frac{\sum_n \lambda_n r_n^2}{2\sum_n r_n^2}. \tag{A14}$$

3. Exact solutions

In this subsection, we find several families of exact solutions of the Toda chain that exhibit different characteristic behavior: "chaotic" $a_n, b_n \propto n$ and "integrable" $a_n, b_n \propto n^{1/2}$. First, we notice that the "center-of-mass" coordinate $\sum_n q_n$ and total momentum $\sum_n \dot{q}_n$ of the Toda chain are free parameters. Hence a transformation $q_n(t) \to q_n(t) + vt + \mathrm{q}$ turns a solution into a solution while transforming

$$a_n(t) \to a_n(t) + v, \quad b_n(t) \to b_n(t). \tag{A15}$$

Since the Toda equations are not explicitly time-dependent, if $q_n(t)$ is a solution, then $q_n(t - t_0)$ for arbitrary t_0 is a also a solution. Finally, rescaling t yields

$$q_n(t) \to q_n(Jt) + 2k\ln(J), \tag{A16}$$

$$a_n(t) \to Ja_n(Jt), \quad b_n(t) \to Jb_n(Jt). \tag{A17}$$

a. "Chaotic" solutions

Keeping these symmetries in mind, we proceed to construct the family of exact solutions as follows: we use the ansatz $b_n^2 = b^2(t)p(n)$, where $p(n)$ is a quadratic polynomial. The constant term in $p(n)$ is arbitrary due to (A15). The overall coefficient can be reabsorbed into b^2, while the constant term is fixed by consistency. The most general solution within this ansatz is $p(n) = (n+c)(n+1)$ with some c. Plugging this into (29), we find

$$\frac{d^2}{dt^2}\ln(b^2) = 2b^2, \quad b^2 = \frac{J^2}{\sin^2(J(t_0 - t))}. \tag{A18}$$

This leads to the solution (30),

$$\begin{aligned} \tau_n &= \frac{G(n+2)G(n+1+c)}{G(c)\Gamma(c)^{n+1}} \frac{J^{n(n+1)}}{\sin(J(t_0-t))^{(n+c)(n+1)}}, \\ q_n(t) &= 2n\ln(J) - (2n+c)\ln(J\sin(J(t_0-t))) \\ &\quad + \ln(n!\Gamma(n+c)), \\ a_n(t) &= (2n+c)J\cot(J(t_0-t)), \\ b_n^2(t) &= \frac{(n+c)(n+1)J^2}{\sin^2(J(t_0-t))}, \end{aligned} \tag{A19}$$

where $G(x)$ is the Barnes gamma function. Positivity of $b_0^2(t)$ requires $c \geqslant 0$.

After taking the limit $J \to 0$ and using the symmetry (A15), the solution becomes

$$\tau_n = \frac{G(n+2)G(n+1+c)}{G(c)\Gamma(c)^{n+1}} \frac{1}{(t_0-t)^{(n+c)(n+1)}}, \tag{A20}$$

$$q_n = -(2n+c)\ln(t_0-t) + \ln(n!\,\Gamma(n+c)), \tag{A21}$$

$$a_n = \frac{2n+c}{t_0-t}, \quad b_n^2 = \frac{(n+c)(n+1)}{(t_0-t)^2}. \tag{A22}$$

The family of solutions (A19) can be further analyzed. We would like to find the explicit form of the orthogonal transformation $Q(t)$. From (A2) it follows that each row of Q, which we (somewhat surprisingly) denote by ψ, will satisfy

$$\dot{\psi}(t) = 2B(2t)\psi(t). \tag{A23}$$

Using the explicit form of $b_n(t)$, we factor out the time dependence of $B(t)$,

$$2B(2t) = \frac{1}{\sin(J(t_0-2t))} 2B(t_i), \quad t_i = t_0 - \frac{\pi}{2J}. \tag{A24}$$

It is convenient to introduce the auxiliary "time" variable $t_M(t)$, which satisfies $dt_M/dt = J/\sin(J(t_0-2t))$,

$$Jt_M = \frac{1}{2}\ln\frac{\cot(J(t_0/2-t))}{\tan(J(t_0/2))}, \tag{A25}$$

such that $t_M(t_i) = 0$. Then $\psi(t_M(t))$ will solve (A23), provided $d\psi/dt_M = 2B(t_i)\psi(t_M)$. Since $a_n(t_i) = 0$, matrix $2B(t_i)$ is related by a simple unitary transformation to $iM(t_i)$. Therefore, up to a trivial factor, $\psi(t_M)$ describes the conventional (Minkowski) time evolution of an operator in Krylov space. This explains the choice of notations for ψ—the "wave-function" of the operator, and t_M—time in Minkowski space. For the system described by Lanczos coefficients $a_n = 0$, $b_n = (n+c)(n+1)$, a particular solution with $\psi_n(0) = \delta_{n0}$ was found in [10],

$$\psi_n(t_M) = (-1)^n\sqrt{\frac{\Gamma(n+c)}{n!\,\Gamma(c)}}\frac{\tanh^n(J\,t_M)}{\cosh^c(J\,t_M)}. \tag{A26}$$

Since $2B(t_i)$ is time-independent, other solutions can be obtained by acting on (A26) by differential operators with constant coefficients, e.g., $\psi^{(1)} = c^{-1/2}\psi'(t_M)$ is a solution satisfying $\psi_n^{(1)}(0) = \delta_{n1}$. After substituting (A25) as an argument of ψ, it becomes the first row of matrix Q,

$$\begin{aligned} Q_{n0}(t) &= (-1)^n\sqrt{\frac{\Gamma(n+c)}{n!\,\Gamma(c)}}\left(\frac{\sin(Jt_0)\sin(J(t_0-2t))}{\sin^2(J(t_0-t))}\right)^{c/2} \\ &\quad\times\left(\frac{\sin(Jt)}{\sin(J(t_0-t))}\right)^n, \end{aligned} \tag{A27}$$

while $\psi^{(1)}$ will become the second row, etc.

From the explicit solution it is easy to see that at $t = t_0/2$ all components of Q_{n0} vanish, while the product $R_{00}Q_{n0}$ is regular. In fact, all components Q_{nm} vanish at $t = t_0/2$. This is easy to see by going back to the "Minkowski" time t_M (A25). When $t \to t_0/2$, $t_M \to \infty$. In this limit, all components of (A26) decay exponentially. Since all rows of Q can be obtained by acting on $\psi_n(t_M)$ by a differential operator with constant coefficients, they all will decay exponentially with t_M and therefore vanish at $t = t_0/2$.

Using the explicit solution (A27) one can easily calculate the inverse participating ratio (37) to immediately conclude that it diverges at $t = t_0/2$. The behavior of (A27) near $t = t_0/2$ is typical, where $t_0 = t^*$ is the point of singularity. To show that, we assume that near $t = t^*$ the tau-function behaves as

$$\tau_0 \propto \frac{1}{(t^*-t)^c}. \tag{A28}$$

Using Hankel determinant representation (A5) we immediately find that the singular behavior of τ_n near $t = t^*$ is given by (A20) with $t_0 = t^*$, from where the singular behavior of q_n, a_n, b_n near $t = t^*$ given by (A21) and (A22) follows.

From the identity $R_{00}(t/2)^2 = \tau_0(t)/\tau_0(0)$ one immediately sees that near $t = t^*/2$, $R_{00}(t) \propto (t^*-2t)^{-c/2}$, and from $R_{00}(t)Q_{00}(t) = \tau_0(t)/\tau_0(0)$ and regularity of $\tau_0(t)$ at $t = t^*/2$ one concludes

$$Q_{00}(t) \propto (t^*-2t)^{c/2}, \tag{A29}$$

near $t = t^*/2$. Now one can use the differential equation for Q (A2), $\dot{Q}_{00}(t) = b_0(2t)Q_{10}(t)$, together with the leading singular behavior of b_0 near $t = t^*/2$ (A22) to conclude that $Q_{10}(t) \propto (t^*-2t)^{c/2}$, and so on.

b. "Integrable" solutions

There is an exact family of solutions $b_n^2 = b^2(t)p(n)$, where $p(n)$ is a linear function of n. Without loss of generality we can choose $p(n) = n + c$, and later see that self-consistency requires $c = 1$. Then $b^2 = e^{m(t-t_0)}$, and

$$\begin{aligned} \tau_n &= G(n+2)e^{\frac{(n+1)}{m^2}e^{m(t-t_0)}}e^{m(n+1)(n+2)(t-t_0)/2}, \\ q_n &= \frac{e^{m(t-t_0)}}{m^2} + (n+1)m(t-t_0) + \ln(n!), \\ a_n &= e^{m(t-t_0)}, \qquad b_n^2 = (n+1)e^{m(t-t_0)}. \end{aligned} \tag{A30}$$

From the positive of b_0^2 it follows that $c \geqslant 0$.

In the limit $m \to 0$, exponent $e^{m(t-t_0)}$ can be expanded in Taylor series, and after rescaling of t one finds

$$\tau_n = G(n+2)e^{n(n+1)/2\ln(a)}e^{a(n+1)(t-t_0)^2/2}, \quad (A31)$$

$$q_n = \frac{a(t-t_0)^2}{2} + n\ln(a) + \ln(n!), \quad (A32)$$

$$a_n = a(t-t_0), \qquad b_n^2 = a(n+1). \quad (A33)$$

Since b_n^2 are time-independent, the differential equation for Q_{n0} is particularly easy to solve,

$$Q_{n0} = \frac{(-a^{1/2}t)^n}{\sqrt{n!}}e^{-at^2/2}. \quad (A34)$$

This is a "wave packet" centered at $n \sim t^2$. It is also easy to calculate the inverse participation ratio (37), $I = e^{2at^2}/I_0(2at^2)$, which grows linearly with t.

Going back to the solution (A30), the "wave function" Q_{n0} is given by (A34) with t substituted by

$$a^{1/2}t \to \frac{e^{-mt_0}}{m}(e^{mt}-1), \quad (A35)$$

which means the inverse participation ratio grows exponentially with t.

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