Solitonlike Structure in the Parametric Distortions of Bounded-System Energy Spectra

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Exact one-soliton and two-soliton solutions of generalized Calogero-Moser (gCM) equations are presented. We explain how these solutions describe the origin of the successive avoided crossings observed in the energy-level structure of bounded systems when a parameter is varied. A new statistical description, based on the grand-canonical ensemble for the gCM system, is developed for the study of the parametric properties of irregular spectra. The relationship with random-matrix theory is discussed.

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In recent years there has been great interest in the properties of avoided crossings in model systems, particularly with respect to their use as a signature of nonseparability. Avoided crossings are displayed in diagrams where the energy spectrum of a system is plotted versus a varying parameter such as the amplitude of an external static electric[1] or magnetic[2] field, or its frequency when the applied field is periodic,[3] or the interatomic distance in a molecule,[4] or the nuclear deformation.[5] Successive avoided crossings along a fictive curve are also observed in many of these diagrams, which suggests the persistence of some property of an eigenstate after several avoided crossings. The purpose of the present Letter is to interpret the nature of avoided crossings from the viewpoint of nonlinear dynamics. To make our arguments specific, we shall consider bounded quantum systems without any special symmetries,[6] and with a Hamiltonian operator which depends linearly on a parameter τ, $\hat{H}(\tau)=\hat{H}_0+\tau\hat{V}$. The energy spectrum of the system is assumed to be discrete, finite, or infinite.

Several recent papers have been devoted to the study of the "motion" (i.e., change) of the eigenvalues and the eigenvectors of $\hat{H}(\tau)$ when the pseudotime parameter τ varies.[7-9] It has been shown that the parametric motion is governed by the generalized Calogero-Moser (gCM) equations, which are the canonical equations associated with the classical Hamiltonian[10]

$$H=\frac{1}{2}\sum_{n=1}^{N}p_n^2-\frac{1}{2}\sum_{m\neq n=1}^{N}\sum_{a,b=1}^{N}\frac{g_m^a f_n^a g_n^b f_m^b}{(x_m-x_n)^2}\,. \qquad (1)$$

In (1), x_n is the nth energy eigenvalue and p_n is the parametric derivative of x_n (also equal to the nth diagonal element of the interacting potential),

$$dx_n/d\tau=p_n=\langle n\,|\,\hat{V}\,|\,n\rangle\,.$$

The nondiagonal elements of $\hat{V}$ are given by

$$\langle m\,|\,\hat{V}\,|\,n\rangle=\frac{\sum_{a=1}^{N}g_m^a f_n^a}{x_m-x_n}\,,$$

where $f_n^a=\langle a\,|\,n\rangle$ and $g_m^a=i\lambda^a\langle m\,|\,a\rangle$, while the $\{\lambda^a,|\,a\rangle\}$ are the eigenvalues and the eigenvectors of the τ-independent operator $\hat{\Lambda}=i[\hat{V},\hat{H}_0]$. The classical Hamiltonian (1) describes the motion of N particles on a line. A pseudospin $\{f_n^a\}$, as well as a pseudocospin $\{g_m^a\}$, is associated with each particle. The particles interact with each other with a repulsive potential.

This system has been shown to be completely integrable when the number of particles is finite.[9,11] Accordingly, it shares the rare feature of integrability with the finite ideal gas, harmonic chain, and Toda chain. Moreover, (1) reduces to the Hamiltonian for a finite ideal gas when $g_m^a=0$. When infinite extensions of their domains are assumed, these latter systems are known to support persistent modes of propagation. In particular, solitons can propagate in the infinite nonlinear Toda lattice. We further develop this analogy by giving here the one-soliton and the two-soliton solutions of system (1).

While the system (1) is completely integrable, neither soliton solutions nor the solution for given initial values have yet been displayed explicitly. In order to construct such solutions, we note that each solution of system (1) corresponds to a parametric family of Hamiltonians of the form $\hat{H}_0+\tau\hat{V}$ and conversely. We therefore consider the following Hamiltonian operator (which has a long history[12]):

$$\hat{H}(\tau)=\begin{bmatrix} p\tau & u_1 & u_2 & u_3 & \cdots & u_N\\ u_1 & y_1 & 0 & 0 & \cdots & 0\\ u_2 & 0 & y_2 & 0 & \cdots & 0\\ u_3 & 0 & 0 & y_3 & \cdots & 0\\ \cdot & \cdot & \cdot & \cdot & \cdots & \cdot\\ \cdot & \cdot & \cdot & \cdot & \cdots & \cdot\\ \cdot & \cdot & \cdot & \cdot & \cdots & \cdot\\ u_N & 0 & 0 & 0 & \cdots & y_N \end{bmatrix}, \qquad (2)$$

where $y_n<y_{n+1}$. The eigenvalues of (2) are given by

the roots of the equation

$$p\tau = x - \sum_{n=1}^{N} \frac{u_n^2}{x-y_n} . \tag{3}$$

Equation (3) possesses $N+1$ roots $\{x_n(\tau)\}$ which generate an exact solution of the system (1). The eigenvalue problem for (2) is thus identical to solving the dynamical system (1) with initial values which are determined from the roots of (3) at $\tau=0$. The energy spectrum is composed of N horizontal levels (i.e., independent of τ) which are crossed by one extra level with a slope given by the parameter p. In fact, each and every crossing is avoided. The repulsion between the levels is controlled by the coupling parameters $\{u_N\}$.[12,13] For equal spacing between the horizontal levels, $y_n = an$, the succession of avoided crossings corresponds to a soliton propagating with a velocity p through a lattice of period a, if the horizontal levels are extended for positive and negative values of coordinate x. The exact one-soliton solution is then given by the zeros $\{x_n(\tau)\}$ of

$$p\tau = x - \frac{\pi u^2}{a} \cot\frac{\pi x}{a} . \tag{4}$$

This formula gives us the soliton profile. At a large distance from the soliton, the decrease of its profile is algebraic, $x_n(\tau) \simeq an + u^2(an - pt)^{-1}$. For the one-soliton solution (4), the velocity of the particles is

$$p_n(\tau) = p\left[1+\frac{\pi^2u^2}{a^2}\left(\sin\frac{\pi x_n(\tau)}{a}\right)^{-2}\right]^{-1} , \tag{5}$$

and the matrix elements of the interaction potential V are then

$$\langle m(\tau)|\hat{V}|n(\tau)\rangle = [p_m(\tau)p_n(\tau)]^{1/2} . \tag{6}$$

The spin and cospin can be obtained as explained above. The velocity (5) decreases at a large distance like $p_n(\tau) \simeq pu|an - p\tau|^{-1}$. Accordingly, the gCM soliton has long-range tails in contrast to the Toda soliton.

Solitons are known to collide with each other without undergoing a change of structure. It is thus important to construct the bisoliton solution of (1) in order to verify this property. The family of Hamiltonian operators we need to consider for this purpose is

$$\hat{H}(\tau) = \begin{bmatrix} q\tau+b & w & v & v & v & \cdots \\ w & p\tau & u & u & u & \cdots \\ v & u & a & 0 & 0 & \cdots \\ v & u & 0 & 2a & 0 & \cdots \\ v & u & 0 & 0 & 3a & \cdots \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdots \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdots \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdots \end{bmatrix} , \tag{7}$$

where u (v) is the coupling between the soliton level with velocity p (q) and the lattice levels, and w is the coupling between the two-soliton levels. The solution is now given by the following quadratic equation in τ:

$$(q\tau+b-x)(p\tau-x)+f(x)[u^2(q\tau+b-x)+v^2(p\tau-x)]-2uvwf(x)-w^2=0 , \tag{8}$$

with $f(x) = (\pi/a)\cot(\pi x/a)$ in the limit of infinite extension. The bisoliton solution is then given by the real roots of Eq. (8). Figure 1 depicts an example of crossing between two solitons, which illustrates their stability with respect to their collision.

Because of their persistence during the avoided crossings, we see that the solitons may be associated with the diabatic energy levels as opposed to the adiabatic energy levels (which are the energy levels themselves). Suppose that the parameter τ varies with time, and that the initial quantum state is one of the energy eigenstates. Then the system will remain on the initial level if the time variation of the parameter is slow. On the other hand, the system will jump from level to level and it will follow the diabatics if the time variation is rapid.[13] This remark establishes the relationship between the different concepts introduced in this Letter and the standard nomenclature of quantum mechanics.

Multisolitons can be constructed by generalization of the above procedure. When many solitons are created in this way, the spectrum appears irregular for any fixed value of the parameter τ. We may then associate an irregular spectrum with an ideal gas of solitons. With this purpose in mind, we must consider the statistical

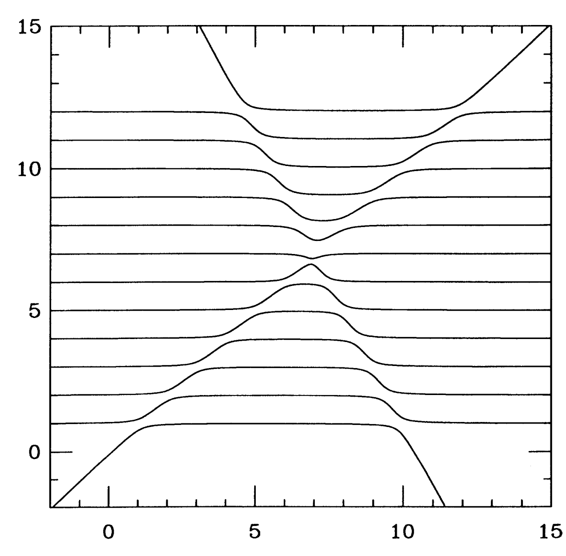

FIG. 1. Example of bisoliton: energy spectrum of the Hamiltonian family (7) with parameter values $p=1$, $q=-2$, $u=0.2$, $v=0.3$, $w=0.4$, $a=1$, $b=21$, and $n=1,2,\ldots,12$.

mechanics of the dynamical system (1).

If the number of solitons in the dynamical system is infinite, statistical concepts are required for its description.[14] To construct an invariant probability measure for the statistical mechanics of system (1), we define a grand-canonical ensemble with a Gibbs measure given formally by

$$dM = \frac{1}{\Xi} e^{-\beta H - \mu N} \prod_{n,a} dx_n\, dp_n\, df_n^a\, dg_n^a , \tag{9}$$

where H is the classical Hamiltonian (1) and N is the number of particles. We give a mathematical meaning to (9) by looking at the system in the finite interval $[-L/2, L/2]$ of the x axis. The number of particles in this interval is a random variable with a Poisson distribution,

$$W_N^L = \frac{(\rho L)^N}{N!} e^{-\rho L} , \tag{10}$$

where ρ is the mean density of levels. For a fixed number N of levels, the probability of a given configuration is obtained by integrating (9) over the variables p_n, f_n^a, and g_n^a. The result is[8]

$$P_N^L(x_1, x_2, \ldots, x_N) = C_N^L \prod_{1 \le i \le j \le N} |x_i - x_j| , \tag{11}$$

which allows us to make a comparison with the predictions of random-matrix theory.[15,16] This latter theory defines statistical ensembles of matrices to study the properties of irregular spectra. The Gaussian orthogonal ensemble, the circular orthogonal ensemble, as well as the Jacobi and the Laguerre orthogonal ensembles,[17] define configuration distributions similar but different from (11). However, all these different ensembles lead to the universal spacing distribution of Mehta, Gaudin, and Dyson (rather than the Wigner distribution).[16,18] Analogously, we can prove that the grand-canonical ensemble defined by (10) and (11) leads to the same universal spacing distribution. The proof makes use of the properties of Legendre polynomials. In this sense we may call the ensemble defined here the Legendre orthogonal ensemble. The equivalence between all these ensembles is a remarkable property, and deserves further study.[18] The assertion on the foundation of random-matrix theory, which was previously based on canonical ensemble,[7] has now been clearer in our treatment based on the grand-canonical ensemble.

The ensemble (9) is useful for the study of the statistical properties of the spectrum itself, and of its parametric distortions. An important parametric property of a spectrum is the level curvature defined as

$$K = \frac{d^2 x_n}{d\tau^2} = -\frac{\partial H}{\partial x_n} , \tag{12}$$

which has been used by several authors[19] to characterize irregular spectra. x_n is an arbitrary level and H is the Hamiltonian (1). K may have positive or negative values. Its probability density is given by

$$P(K) = \lim_{N \to \infty} \int \delta \left(K + \frac{\partial H}{\partial x_1} \right) dM = \lim_{N \to \infty} \sum_{a=2}^{N} \int \left| \frac{\partial^2 H}{\partial x_1^2} \right|^{-1} \delta[x_1 - x_1^a(K)]\, dM , \tag{13}$$

where dM is the measure (9) and $\{x_1^a(K)\}$ are the $N-1$ zeros of $K + \partial H/\partial x_1 = 0$. $P(K)$ can be evaluated asymptotically for large K. We obtain

$$P(K) \sim \frac{1}{|K|^{\nu+1}}, \quad |K| \to \infty , \tag{14}$$

with $\nu = 1$. In general, we expect that the curvature density will decrease like (14) if the spacing density behaves like S^ν ($\nu = 1,2,4$) near $S = 0$. The different universality classes of spectra can thus be distinguished by the curvature distribution, which is to be considered a parametric property. This universality can be evaluated by numerical diagonalization of Hamiltonian operators, as well as deduced from experimental data. Other parametric properties could also be studied using the statistical ensemble (9), e.g., the mean-square displacement of an energy level when the parameter is varied, or the parameter-dependent structure function $S(k,\tau)$.[20] These properties were studied in the Brownian-motion model of Dyson,[21] for which the present formalism provides complete justification.

Random-matrix theory is only useful for studying irregular spectra when the parameter is fixed once and for all. On the other hand, the statistical ensemble we have defined with the parametric Hamiltonian (1) allows us to study irregular spectra for fixed and variable values of the parameter τ. In this sense, the present theory generalizes random-matrix theory. Similar considerations hold for quantum dissipative systems.[22]

To conclude, we have shown the exact soliton solution which can be observed in an energy spectrum when a parameter is varied. We suggest that the soliton description of parametric distortions of spectra will allow investigation of the ergodic properties of the parametric system (1). Many tools accumulated in the field of nonlinear dynamics of solitons will be extremely useful in this context.

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