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Nonintegrability and quantum spin chains

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This study concerns the concept of nonintegrability in quantum many-body systems, which is related to the important and unresolved problem of quantum chaos. Our findings strongly indicate that nonintegrability affects the reliability of many approximation techniques which have proved to be successful in the study of integrable models. This report is based on finite-size studies of the low-lying spectral excitations of both integrable and nonintegrable 1D quantum spin models. In integrable cases, the characteristic excitation pattern of the infinite system is apparent even in relatively short chains. This is generally not the case in nonintegrable systems where we observe several classes of excitations with qualitatively different character. In some situations, the nature of the lowest-lying excitations actually changes with increasing system size, which makes finite-size studies very vulnerable to misleading conclusions if care is not taken.

Conformal invariance has indicated the existence of infinite classes of integrable models in statistical mechanics.[1,2] The discovery of this principle has focused attention on the concept of integrability in classical and quantum many-body systems. It is well known that the role of integrability is quite striking in the behavior of classical dynamical systems. The dynamical properties of *integrable* systems undergo drastic changes if subjected to *nonintegrable* perturbations, giving rise to qualitatively new phenomena, which are well described by the theory of deterministic chaos.[3] This raises a question of considerable interest: what are the implications of integrability and nonintegrability for *quantum* many-body systems, and what is the relation to the important and unresolved issue of quantum chaos?[4] Interacting spin systems provide convenient models for the study of nonintegrability effects in both classical and quantum mechanics.[4–7] A recent study of the nature of quantum chaos in spin systems has put the various concepts of integrability for classical and quantum spin systems into perspective.[4]

For a system of N localized classical three-component spins $\mathbf{S}_l$, $l = 1,...,N$ specified by some interaction Hamiltonian $H(\mathbf{S}_1,...,\mathbf{S}_N)$ there are two concepts of integrability in use: *Dynamical integrability*: A system of N classical spins is dynamically integrable (completely integrable, separable) if there exist N distinct integrals of the motion in involution.[3,4,6,7] *Thermodynamic integrability*: A classical spin system is thermodynamically integrable (exactly solvable) if it is possible to determine its partition function

$$Z_N = \int d\,\mathbf{S}_1 \cdots \int d\,\mathbf{S}_N\, e^{-\beta H(\mathbf{S}_1,...,\mathbf{S}_N)} \tag{1}$$

exactly in the thermodynamic limit $N \to \infty$. Whereas thermodynamic integrability depends on the energy function $H(\mathbf{S}_1,...,\mathbf{S}_N)$ alone, the concept of dynamical integrability further depends on the specification of the Poisson brackets for classical spin variables (the symplectic structure), which determine their time evolution via the Hamilton equation of motion. Dynamical nonintegrability may be realized for N as low as $N = 2$,[6,7] but effects of thermodynamic nonintegrability only in the thermodynamic limit. The existence of an infinite set of conservation laws lies at the heart of any method to determine the thermodynamic properties of an infinite classical spin system, most conspicuously in the solutions based on the diagonalization of the transfer operator. The infinite quasi-degeneracy in the vicinity of the largest eigenvalue of the transfer operator is a crucial prerequisite for the standard critical behavior at a continuous phase transition with all the well-known scaling properties. Whether all the scaling properties continue to hold in thermodynamically nonintegrable models is an important unresolved problem.[4,8] It is related to the phenomenon of quantum chaos in many-body systems, and this report is based on our current comprehensive investigation of quantum chaos.

In contrast to classical spin systems, there is only a single concept of integrability for quantum spin systems, which relates to both thermodynamic and dynamical properties. Model systems containing a finite number of interacting quantum spins are always integrable, at least in principle. Since the underlying Hilbert space has finite dimensionality, $(2s+1)^N$, the time evolution of any quantity is at most multiperiodic. Nonintegrability effects in quantum spin systems are therefore expected to appear only in either of the following two limits: Classical limit: N finite, $s \to \infty$. Thermodynamic limit: s finite, $N \to \infty$. Nonintegrability effects observed in small quantum spin clusters for large s can be regarded as precursors of classical dynamical chaos.[4] Nonintegrability effects observed in quantum spin chains for large N, on the other hand, may be interpreted as manifestations of quantum chaos and are the focus of this report. Since chaotic phenomena associated with nonintegrability are most dramatically apparent in dynamical as opposed to static properties, one might wish to study primarily the dynamical properties of quantum spin chains. The problem is that dynamical properties of such systems are highly nontrivial

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even for integrable models,[9] which makes it very difficult to identify nonintegrability effects there (see Ref. 4 for specific predictions). Here, we focus instead on unusual effects in the spectral properties of nonintegrable quantum spin chains, particularly in the spectrum of low-lying excitations.

We have investigated analytically and numerically a variety of integrable and (apparently) nonintegrable 1D spin models. Integrable 1D quantum spin models include, most prominently, the class of Bethe-ansatz solvable models such as the 1D $s = 1/2$ Heisenberg model

$$H = J \sum_{l=1}^{N} \mathbf{S}_l \cdot \mathbf{S}_{l+1} \tag{2}$$

and some of its generalizations, such as the 1D $s = 1/2$ XXZ model

$$H = J \sum_{l=1}^{N} (S_l^x S_{l+1}^x + S_l^y S_{l+1}^y + \Delta S_l^z S_{l+1}^z) \tag{3}$$

and the 1D $s = 1$ bilinear-biquadratic model[10]

$$H = J \sum_{l=1}^{N} [\mathbf{S}_l \cdot \mathbf{S}_{l+1} - (\mathbf{S}_l \cdot \mathbf{S}_{l+1})^2], \tag{4}$$

or the 1D $s = 1/2$ anisotropic XY model

$$H = J \sum_{l=1}^{N} [(1+\gamma) S_l^x S_{l+1}^x + (1-\gamma) S_l^y S_{l+1}^y] \tag{5}$$

which maps onto a free-fermion system.

We have studied these models subjected to nonintegrable perturbations by looking at finite-chain sequences, by calculating in some cases all eigenstates, and by using Lanczös techniques to obtain results for special states of interest at larger N. Nonintegrability effects resulting from the absence of a sufficient number of conservation laws are expected to make their appearance in the form of an increasing level turbulence for increasing N, which would manifest itself, for example, in the form of changes in trend in extrapolations with $1/N$, in the failure of expected scaling behavior and in the presence of unusual classes of excitations. In the following, we summarize a number of observations which are difficult to categorize in terms of familiar phenomena in integrable models.

The $s = 1/2$ XY model: response to an in-plane magnetic field. Consider the integrable model described by Hamiltonian (5) with $\gamma = 0$. The addition of a Zeeman term $-h \sum_l S_l^x$ makes it nonintegrable. Two numerical methods have been used to calculate the $T = 0$ in-plane susceptibility χ_{xx} for $h = 0$. One method was a $T = 0$ Padé analysis of exact results for $\chi_{xx}^{(N)}$ for finite chains with up to $N = 10$ spins, yielding the extrapolated value $J\chi_{xx}^{(\infty)} \simeq 0.055$.[11] An alternative approach based on extrapolations of $T > 0$ calculations of $\chi_{xx}^{(N)}$ for $N = 2,...,10$, yielded the very different value $J\chi_{xx}^{(\infty)} \simeq 0.117$.[12,13] The lack of consistency of these numerical approaches is unprecedented in its extent and most puzzling in the light of numerical studies of the $T = 0$ susceptibility χ_{xx} for the $s = 1/2$ Heisenberg chain, Eq. (2), where the results of various numerical approaches were in reasonable agreement with each other and with the exact result.[14,15] The exact result $J\chi_{xx} = 0.075\,566...$ for the XY model, on the other hand, which was calculated from exactly known dynamic correlation functions in the integrable limit $h = 0$,[16] proved to be in poor agreement with any of the numerical predictions. While it is true that a square-root cusp singularity is present in the wave-number dependent susceptibility $\chi_{xx}(q)$ at $q = 0$, which might tend to slow numerical convergence, the observed discrepancies of over 50% are much too large to ascribe solely to this cause.

The spin-s XYZ model: Haldane prediction. Some time ago, Haldane made the challenging prediction that the $T = 0$ phase behavior of the spin-s XXZ model (3) as a function of Δ is qualitatively different for integer s and half-integer s.[17] Substantial evidence has accumulated in support of Haldane's picture as a result of several numerical studies. However, some puzzling results have also appeared which have in common the fact that they do not appear in known integrable models. Specifically they are absent in the Bethe-ansatz solvable $s = 1/2$ XXZ chain but not in $s > 1/2$ XXZ chains of either integer *or* half-integer s. Examples appear below.

Spin-s Heisenberg chains: spectral crossover in a magnetic field. The dispersion curves of low-lying excitations for the Heisenberg chain are well known to have a qualitatively different magnetic-field behavior in the $s = \frac{1}{2}$ case (quantum limit, Bethe ansatz) and in the $s = \infty$ case (classical limit, linear spin-wave theory). The $s = \frac{1}{2}$ dispersion curves are most prominently characterized by the existence of two distinct zero-frequency modes, one at $q = 0$ and one at $q = 2\pi M$, where $0 \leqslant M(h) \leqslant \frac{1}{2}$ is the $T = 0$ magnetization as a function of the external magnetic field.[18,19] This latter soft mode, which tracks across the Brillouin zone as h increases from zero to the saturation value $h_c = 2J$, has no counterpart in the classical spectrum. This raises the interesting question as to how the quantum spectrum is transformed into the classical spectrum for increasing. A detailed finite-chain study of the $s > \frac{1}{2}$ Heisenberg models, which apparently are nonintegrable, has revealed that the spectra of low-lying excitations fall into two distinct classes.[19] Excitations with quantum number $S_T^z \equiv \sum_l S_l^z = Ns, Ns - 1,...,Ns/2$ do exhibit the tracking soft-mode characteristic of the integrable $s = \frac{1}{2}$ Heisenberg chain. Whereas for $s = \frac{1}{2}$ all low-lying excitations belong to this category for the entire field range $h = 0$ to $h = h_c$, this is not so for $s > \frac{1}{2}$, where this type of excitation dominates the low-energy spectrum only in a smaller h-interval adjacent to h_c, whose size shrinks with increasing s. The second class of excitations, with quantum number $S_T^z = Ns/2, Ns/2 - 1,...,0$, displays a qualitatively different spectral behavior, which is more reminiscent of the classical spin-wave dispersion curves. Therefore, the spectrum of low-lying excitations undergoes a very peculiar crossover for increasing h, which is completely different from anything observed in exactly solved models.

Consider, for example, the bilinear-biquadratic Hamiltonian (4) which describes the *integrable* spin-1 model most closely related to the spin-1 Heisenberg model (2), and which is, in fact, just one member of a general class of Bethe-ansatz solvable models for general spin s whose Hamiltonians have the general structure of a polynomial of degree $2s$ in $\mathbf{S}_l \cdot \mathbf{S}_{l+1}$.[10] All members of this integrable family, which includes the $s = \frac{1}{2}$ Heisenberg model, show qualitatively the same $T = 0$ phase behavior as a function of the external magnetic field. It is a characteristic of integrable systems that the general character of any particular class of low-lying excitations is apparent even for relatively short chains, a feature which has been explicitly observed in all integrable models mentioned in this paper, but which is conspicuously absent in the $s > \frac{1}{2}$ Heisenberg chains. In particular, the excitation spectra of the integrable models do not exhibit the peculiar crossover phenomenon observed in the $s > \frac{1}{2}$ Heisenberg chains.

The generalized bilinear-biquadratic model. If we take the spin-1 bilinear-biquadratic model of Eq. (4) and insert a variable parameter β multiplying the biquadratic term, we obtain a generalized spin-1 model with the following special limits: the Heisenberg antiferromagnet is specified by the point $\beta = 0$, the integrable Russian model by the point $\beta = 1$ and the model with purely biquadratic exchange by the limit $\beta \to \infty$. By using techniques of conformal invariance, Affleck[20] predicted that as the parameter β moves away from the Russian point $\beta = 1$, a gap opens in the excitation spectrum of this model. The Affleck prediction has been examined by means of scaled-gap,[21] finite-size scaling,[22] and general finite-chain studies.[23] An unusual crossover phenomenon, not previously encountered in finite-size scaling calculations, occurs in the Russian-biquadratic regime. Studies have revealed the presence of singlet excitations[21,22] which appear to extrapolate to zero over the entire range $\beta > 1$. In fact, the lowest singlet excitation lies lower than the lowest triplet excitation for $N \geqslant 8$ at $\beta^{-1} = 0$, for $N \geqslant 10$ at $\beta^{-1} < 0.2$ and for $N \geqslant 12$ at $\beta^{-1} < 0.3$. Here we have a model in which not even the character of the lowest excitations can reliably be identified unless the detailed spectrum is scrutinized for relatively large systems.[21,23] No such phenomenon has ever been observed in integrable models.

"*Supersoft*" *modes at the Heisenberg point* ($\beta = 0$). A similar phenomenon seems to occur in the Heisenberg limit ($\beta = 0$) of this general spin-1 model. The predicted Haldane gap has been investigated numerically almost exclusively for the "primary" excitation gap involving a singlet ground state at wave number $k = 0$ and a triplet excitation at $k = \pi$. The estimated size of the gap is quite large, namely $\Delta E / J \sim 0.41$.[24] However, an unusual class of excitations starts to become prominent for $N \geqslant 12$. Their origin and significance was not known at the time. In the case of the spin-1 *XXZ* model for values of anisotropy Δ near the Heisenberg point $\Delta = 1$, these modes appear to extrapolate with $1/N$ to values *significantly below* the corresponding extrapolations for the primary singlet-triplet gaps. In the Heisenberg limit, they may even extrapolate to zero.[24] These are modes of intermediate k, and therefore finite-size effects are expected to be more pronounced. However, since they apparently have the potential for a radical modification of the accepted phase diagram for the $s = 1$ *XXZ* model, these modes should receive further investigation.

In summary, we have identified several unusual effects in the excitation spectrum of nonintegrable 1D quantum spin models which have not been observed in integrable quantum chains. We conclude that numerical studies of such models must proceed with extreme caution to avoid misleading conclusions. Some of the phenomena reported in this paper might be interpreted as precursors of quantum chaos, which is truly manifest only in the thermodynamic limit.

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