Level repulsion in integrable and almost-integrable quantum spin models

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The repartition of the separation between energy levels of various isotropic $S = \frac{1}{2}$ antiferromagnetic chains is studied numerically with the aim of investigating the transition from integrable to nonintegrable systems. We begin by displaying the level separation distribution of the integrable Bethe chain. Then two nonintegrable systems, two coupled chains, and a next-nearest-neighbor coupled chain, are studied as a function of the coupling. We examine how the level spacing evolves from the Poisson distribution to the Gaussian-orthogonal-ensemble distribution. Finally we consider the Haldane-Shastry $1/r^2$ model. A number of conclusions regarding the behavior and relevance of the level-spacing distribution in these spin systems is drawn.

I. INTRODUCTION

Interest in strongly interacting fermion systems has recently been invigorated with the discovery of high-temperature superconductors. Another strongly interacting fermion system is the atomic nucleus. The stability of nuclei and description of their low-energy excitations have been understood for many years. But the higher-energy excited states of the nucleus are complex and can only be described statistically. Wigner[1] suggested that the Hamiltonian of this system should be similar to a random matrix and that the distribution of spacings of nuclear energy levels should reflect this.[2,3] In particular the Gaussian orthogonal ensemble (GOE) of $N \times N$ real symmetric matrices, invariant under orthogonal transformations, with random matrix elements that are Gaussian distributed [zero mean, variance v^2 (diagonal elements have variance $2v^2$)] has the following properties.

(a) The ensemble-averaged density of states has the elliptical form[4] $\rho(x) = \sqrt{4-x^2}/2\pi$, where $x = E/\sqrt{Nv^2}$, $|x| < 2$, and zero otherwise. This is referred to as Wigner's semicircle law.

(b) The probability that the eigenvalues are $\lambda_1, \ldots, \lambda_N$ is[5]

$$P(\lambda_1, ..., \lambda_N) = \frac{2^{N(N-1)/4}}{n!(2v)^{N(N+1)/2}\prod_{g=1}^{N}\Gamma(\frac{g}{2})} \times e^{-\sum_i \lambda_i^2/4v^2} \prod_{i,j} |\lambda_i - \lambda_j|. \quad (1.1)$$

The last term in the above equation gives rise to energy level repulsion. The distribution of spacings between pairs of energy levels has been found empirically to be quite accurately described by the "Wigner surmise"[1] based on two-dimensional matrices. This surmise is that the probability that the spacing between two adjacent levels is s is $P(s) = (s\pi/2)\exp(-s^2\pi/4)$, where the probability has been normalized so that $\langle s \rangle = 1$.

In contrast, integrable systems, which have as many constants of the motion as degrees of freedom, and for which each energy level can be labeled by that many quantum numbers, have generically a Poisson distribution $P(s) = e^{-s}$ for the energy-level spacing.[6] The Hamiltonians of these systems can be thought of as being representable by random *diagonal* matrices. The interpolation between Poisson and GOE distributions has been modeled by so-called "band random matrix ensembles" (BRME's).[7] In these ensembles only the off-diagonal elements in some sense "close" to the diagonal are nonzero and random. This is meant to interpolate between the random diagonal matrix and the GOE in which all off-diagonal elements are nonzero and random. A BRME might be relevant for local tight-binding models since in a natural basis of states (e.g., the one that is diagonal in S_i^z, for all sites i) only a few entries will have a nonzero value. On the other hand the nonzero matrix elements will be scattered about and not all close to the diagonal. Moreover, expressing the Hamiltonian in a basis where all the obvious symmetries are also diagonal will leave us with a block-diagonal matrix where all the blocks will have only nonzero entries (particularly when we diagonalize with respect to total spin). Therefore we do not see how to justify using the BRME to interpret our results.

The theoretical motivation for the studies undertaken here and by Montambaux *et al.*[8] is the search for a microscopic theory of high-temperature superconductors. In the "normal" state of these materials they are not Landau-Fermi liquids.[9] One of the challenges in the field is to prove or disprove the existence of a Fermi liquid in two-dimensional interacting electron models. In a Landau-Fermi liquid the momenta and spin $\{k_i, \sigma_i\}$ of excited quasiparticles form a set of good quantum numbers. Those who have modeled high-temperature superconductors by a strongly interacting model such as the large-U Hubbard model or t-J model and tried to construct elementary single-particle excitations have not had success in constructing elementary quasiparticle excitations which are weakly interacting.

In one dimension, Fermi-liquid behavior and the set of momenta, charge, and spin of Landau quasiparticles may be replaced by the integer parameters of a Bethe

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ansatz solution of an interacting model (if one exists). If this does not happen in two dimensions, how then might Landau–Fermi-liquid behavior disappear? It has been proposed[10] that perhaps there *do not exist* weakly interacting quasiparticles whose momenta, charge, and spin would be a "good" set of quantum numbers. In that case, the absence of "good" quantum numbers might be signaled by level statistics resembling those of random matrices. If, on the other hand, an interacting fermion system retained Landau–Fermi-liquid behavior one might expect to see the level statistics of an integrable system, especially for low-energy excitations. The first numerical study along these lines was performed by Montambaux *et al.*[8] who showed that a special case of the doped t-J model has a level distribution agreeing quite well with that of the GOE.

In order to investigate the transition between integrability and nonintegrability we have studied the energy-level spacing in two integrable quantum spin systems and related, but nonintegrable, models which may be obtained from an integrable one by tuning a single parameter. The primary integrable model we worked with was the $S = 1/2$ antiferromagetic chain. This model is well studied and enables us to compare the behavior of the level separation distribution with the known properties of this system as it is perturbed.

II. NUMERICAL PROCEDURE

For simplicity and clarity we chose to work with isotropic spin systems. In this case the total spin and total S^z are good quantum numbers. It is only necessary to consider the subspace $S^z = 0$ which contains all of the eigenenergies. Open boundary conditions were chosen. The eigenstates are representations of the trivial spatial symmetries, namely, reflection and rotation in spin space. Thus they can be grouped according to their respective quantum numbers, parity P, and total spin S. The perturbations which carry the system from an integrable to a nonintegrable one will always respect the trivial spatial symmetries. States in different (P, S) sectors will never be coupled and their energy levels never correlated. Thus we calculate the energy-level separation distribution within each (P, S) sector separately. In order to obtain good statistics one requires a large number of states in each (P, S) sector. It was for this reason that periodic boundary conditions for the spin chain were not used. In that case the parity under reflection, P (which takes the values ± 1), would be replaced by momentum which takes on L values, where L is the length of the chain.

The Hamiltonian was diagonalized numerically using the Jacobi method. States were sorted by energy, S, and P. In order to correct for gross variations of the density of states as a function of energy the level spacing was normalized by the smoothed local density of states. This process is commonly referred to as unfolding the spectrum to remove a fluctuating local level density. This was performed for each set of quantum numbers separately. In general this did not affect the level-spacing distribution very much at all as the density of states was generally constant with a falloff at the "band" edges. The states with energies near the band edges were discarded by dividing the states of each (P, S) sector into ten bins ordered by energy and of equal width. The states of the first and last bins were then discarded. In order to compare with the statistical distributions, the energy-level separations were normalized to have a mean of unity. After discarding results from (P, S) sectors with less than 50 states (generally the high-spin sectors) the results of remaining sectors were combined at this point in order to improve the statistics. We checked that all of the sectors had roughly the same behavior. The probability function $P(s)$ was plotted by binning the data and again normalizing the number of states in each bin so that $\int P(s)ds = 1$. In some cases $I(y) = \int_0^y P(s)ds$ was calculated so that this last binning step could be skipped.

It is useful to know, given the typical size of the Hamiltonian matrix (after sorting by the straightforward symmetries), how well the level spacings of the eigenvalues of a random matrix of that size follow the Wigner surmise. The linear matrix dimensions encountered in this work are in the range 100–500. Although this sort of calculation has been published in the past,[2] we have redone such a calculation and in Fig. 1 we show the $P(s)$ obtained (by the method described above) with the matrices of the same size as encountered in the (P, S) sectors of an open $L = 14$ site chain. Figure 1 shows the level of "noise" expected even if the random matrix hypothesis is satisfied. Also shown is the "noise" level expected upon comparing $P(s)$ of random diagonal matrices of these sizes to a Poisson distribution.

III. BETHE CHAIN

We begin by examining the familiar $S = 1/2$ antiferromagnetic chain on L sites with nearest-neighbor coupling,

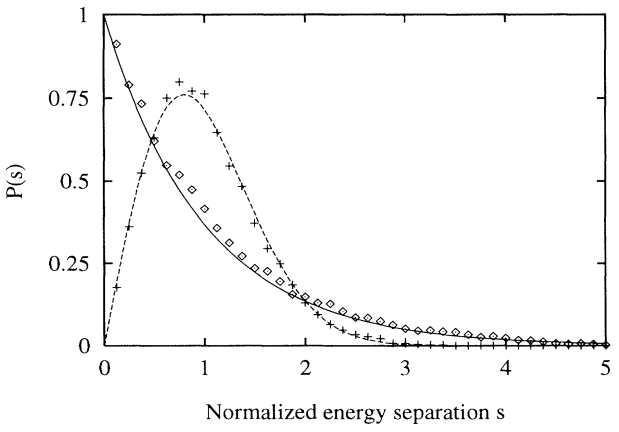

FIG. 1. Level-spacing distribution calculated using random symmetric matrices (with Gaussian distributed elements) and random diagonal matrices of the sizes encountered in the 14-site chain. Solid curve, Poisson distribution; long-dashed curve, Wigner surmise; diamonds, random diagonal matrices; plus signs, random symmetric matrices.

$$H = \sum_{i=1}^{L-1} J\mathbf{S}_i \cdot \mathbf{S}_{i+1}. \quad (3.1)$$

This model remains integrable with our choice of open boundary conditions. In Fig. 2 we show $P(s)$ for chains of length $L = 12$ and $L = 14$ ($L = 13$ is similar but for clarity it is not shown). They are compared with the Poisson distribution and Wigner's surmise for the GOE. Consistent with the integrability of this system the agreement with the Poisson distribution is good, especially in the tail. There is a small deviation from the Poisson distribution at intermediate s which is more than that of random diagonal matrices of similar dimensions. The comparison of the $L = 12$ and $L = 14$ cases gives an idea of finite-size effects which may explain this deviation.

IV. TWO COUPLED CHAINS

In this section we consider two open chains. They are coupled by a simple nearest-neighbor interaction,

$$H = \sum_{i=1}^{L-1}\sum_{j=1}^{2} J\mathbf{S}_{i,j} \cdot \mathbf{S}_{i+1,j} + \sum_{i=1}^{L} J_\perp \mathbf{S}_{i,1} \cdot \mathbf{S}_{i,2}, \quad (4.1)$$

where $j = 1, 2$ is the chain index. An additional symmetry, reflection between chains, appears and so the eigenstates were also sorted by parity under this reflection. For zero coupling the system is integrable and when coupling is turned on the system is not integrable (in fact our calculation erases any doubt that this system might have been integrable). Such a coupling between two chains is believed to be a relevant perturbation for the ground state.[11] We studied this system with the hope that perhaps the relevance or irrelevance of the interchain coupling might be apparent in the level-spacing distribution. That is, if the coupling were irrelevant, the spectrum would look like that of two integrable chains. If the coupling were relevant, then the spectrum would look like that of an nonintegrable system.

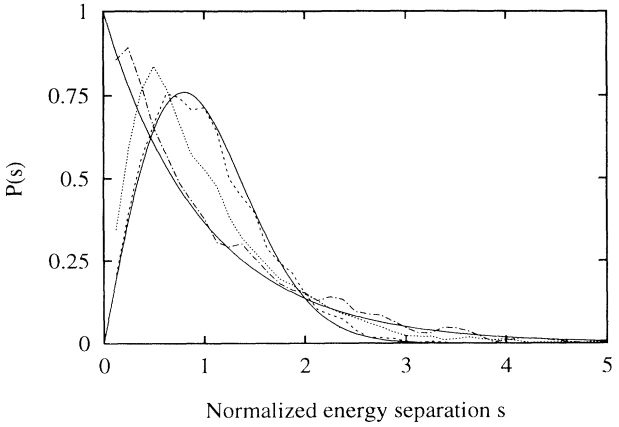

FIG. 3. Level-spacing distribution for two coupled chains each of length 7 for different interchain couplings. The points have been joined for clarity. Medium-dashed curve, $J_\perp/J = 1.0$; short-dashed curve, $J_\perp/J = 0.1$; dot-dashed curve, $J_\perp/J = 0.01$.

The distribution $P(s)$ for two chains of length $L = 7$ is plotted in Fig. 3 for various values of $J_\perp/J$. There is an evolution from a Poisson distribution to the Wigner surmise as $J_\perp/J$ is turned on. In order to quantify the evolution between these two distributions we shall describe it by the single parameter[12] $I = \int_0^\eta P(s)ds$, where $\eta \approx 2.002$ is the greater of the two values of s where the Poisson and GOE distributions cross. At the crossing point, I is most sensitive to the difference between Poisson and GOE distributions. For the Poisson and GOE distributions, I has the values 0.8649 and 0.9571, respectively.

In Fig. 4, I is plotted as a function of $\ln(J_\perp/Jd)$ separately for the values $S = 0, 2, 4, 6, 8$ of total spin. The parameter Jd is the average spacing between energy levels for a given value of S. It was extracted from our numeri-

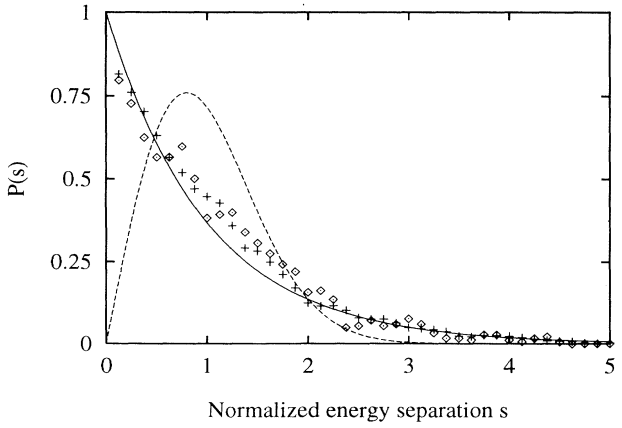

FIG. 2. Level-spacing distribution for the 12-site and 14-site $S = 1/2$ antiferromagnetic chains with open boundary conditions. Diamonds, $L = 12$; plus signs, $L = 14$.

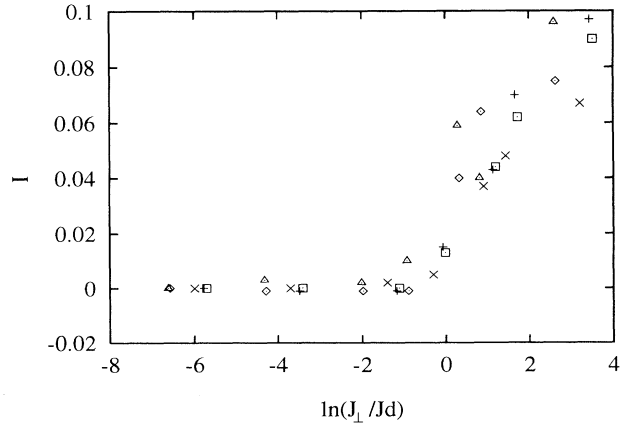

FIG. 4. Interpolation parameter I as a function of interchain coupling $\ln(J_\perp/Jd)$. Diamonds, $S = 0$; plus signs, $S = 2$; squares, $S = 4$; crosses, $S = 6$; triangles, $S = 8$.

cal results. We subtracted the (empirical) small-$J_\perp$ limit of I before plotting because I did not converge to the ideal Poisson distribution value of 0.8649 (probably due to finite-size effects). Figure 4 shows that the transition from Poisson to GOE is roughly the same in the different spin sectors averaged to arrive at Fig. 3. Our results are consistent with the idea that, in general, level repulsion will be fully developed when the typical energy shift due to a perturbation is of the order of the typical spacing between unperturbed energy levels. For two chains of length $L = 7$, the average level spacing of the large sectors ranges from 0.03 to 0.07 J. The expectation value of the $J_\perp$ perturbation is difficult to estimate, but there are seven links between the two chains and the rough order of magnitude of $\langle \mathbf{S}_{i,1} \cdot \mathbf{S}_{i,2} \rangle$ should be 1/4. Thus before $\ln(J_\perp/Jd)$ reaches -1 or so level repulsion should have set in. This is observed and so our results are consistent with a transition to nonintegrability for arbitrarily small $J_\perp/J$ in the thermodynamic limit. Another fact supporting the idea of comparing mean energy spacings with the size of the perturbation is that the level-spacing distributions are roughly similar if one changes the sign of $J_\perp$.

V. NEXT-NEAREST-NEIGHBOR-COUPLED CHAIN

We now consider a chain with next-nearest-neighbor (NNN) coupling,

$$H = \sum_{i=1}^{L-1} J\mathbf{S}_i \cdot \mathbf{S}_{i+1} + \sum_{i=1}^{L-2} J_2 \mathbf{S}_i \cdot \mathbf{S}_{i+2}. \tag{5.1}$$

For $J_2/J = 0$ this system is of course integrable. Near $J_2/J = 0.24$ it is believed that the ground state of this system undergoes a transition from a liquidlike to a dimerlike ground state.[13] At $J_2/J = 0.5$ the ground state is known,[14] and is simply the (doubly degenerate) dimer solid. It would be interesting to see if this qualitative behavior of the ground state is at all reflected in the level-spacing distribution $P(s)$. One factor which may be significant is the proximity of the integrable $1/r^2$ model,[15] which is discussed in the following section.

In Fig. 5 we plot $P(s)$ for a number of values of J_2/J with $L = 13$. There is no special behavior near the point $J_2/J = 0.24$ except that level repulsion settles in continuously but more slowly (as a function of J_2 or $J_\perp$) than for the coupled-chain problem. To illustrate this explicitly we plot the parameter I versus $\ln(2J_2/Jd)$ in Fig. 6. Subtracted from I is its empirical value when $J_2 = 0$. Jd is again the observed average level spacing which is different for sectors of different total spin. The extra factor of 2 appears because NNN coupling introduces one coupling per site whereas in the interchain coupling problem there is one extra coupling for every two sites. Comparing Fig. 4 to Fig. 6 one sees that the parameter I starts to deviate from its value for the integrable case at a larger value of $\ln(2J_2/Jd)$ than $\ln(J_\perp/Jd)$ for coupled chains. So in terms of affecting integrability it would seem that

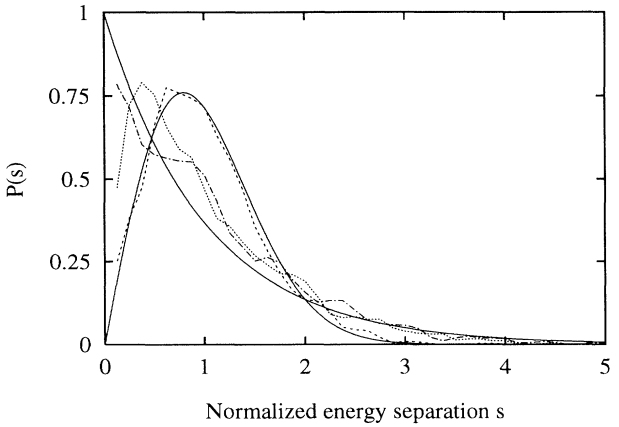

FIG. 5. Level-spacing distribution for the next-nearest-neighbor-coupled antiferromagnet for various couplings. Medium-dashed curve, $J_2/J = 1.0$; Short-dashed curve, $J_2/J = 0.3$; dot-dashed curve, $J_2/J = 0.1$.

interchain coupling is a somewhat stronger perturbation than NNN coupling. This behavior is also evident upon examining the whole integrated probability distribution curves $I(y) = \int_0^y P(s)ds$ for these models.

Another way of understanding the above observation is that the resistance to level repulsion might be due to the proximity of the integrable $1/r^2$ model [Eq. (6.1)]. When $J_2/J = 0.25$ the Hamiltonian 5.1 contains the first two terms of Eq. (6.1). In order to test this idea we evaluated the level-spacing distribution for a *ferromagnetic* ($J_2/J < 0$) coupling. We found that the level-spacing distribution as a function of $|J_2/J|$ behaved essentially the same as for antiferromagnetic NNN coupling. So the proximity of the $1/r^2$ model is perhaps not responsible. Another, less likely, possibility is that there is a hitherto unknown integrable model nearby with ferromagnetic NNN coupling.

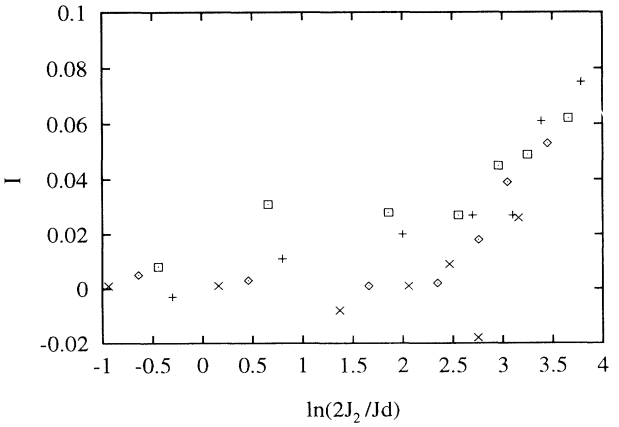

FIG. 6. Interpolation parameter I as a function of next-nearest-neighbor coupling $\ln(2J_2/Jd)$. Diamonds, $S = 1$; plus signs, $S = 3$; squares, $S = 5$; crosses, $S = 7$.

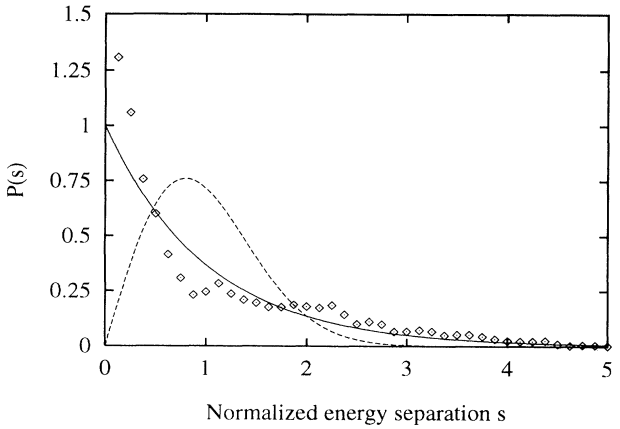

FIG. 7. Level-spacing distribution for the 13-site $1/r^2$ antiferromagnet.

VI. $1/R^2$ CHAIN

The spin-1/2 periodic chain with Hamiltonian

$$H = \sum_{i,n} \frac{J}{2} \sin^{-2}(n\pi/L) \mathbf{S}_i \cdot \mathbf{S}_{i+n} \tag{6.1}$$

was studied by Haldane[15] and Shastry[15] and shown to be integrable. We have studied an open chain version

$$H = \sum_{i,j=1;i\neq j}^{L} \frac{J}{2} |i-j|^{-2} \mathbf{S}_i \cdot \mathbf{S}_j \tag{6.2}$$

in order to avoid the appearance of L conserved momenta which would reduce the statistical significance of the level-spacing distribution. The results for a chain of length $L = 13$ are summarized in Fig. 7. The level-spacing distribution is strikingly unusual in that the probability of closely spaced levels is *larger* than for a Poisson distribution. One way that this might arise is through the Landau levels of an external magnetic field, but no such field is present here. It would be interesting to know if recent advances in understanding this model[16] could explain this behavior.

VII. CONCLUSIONS

In this work we have studied the level-spacing distribution for interacting quantum many-body systems represented by antiferromagnetic spin-1/2 chains. We have confirmed that the level-spacing distribution for the integrable Bethe chain is Poissonian and that certain perturbations lead to level repulsion. A system was found, the $1/r^2$ model, which displays level attraction. We were able to track the transition from integrability to nonintegrability. We conclude, by a small system diagonalization, that certain systems such as two coupled chains or the NNN coupling model (irrespective of the sign of coupling) are definitely *not* integrable. A possible problem which did not appear was that of a long chain "almost" having translation invariance and hence an "almost" good momentum quantum number. That would introduce additional degeneracies in the nonintegrable models, but none were seen.

Level repulsion seems to set in, as one might guess, when the perturbation is of the same size as the typical spacing between energy levels. In the thermodynamic limit the extension of this idea would require some care. One would need to scale both the energy-level spacing and perturbation with system size. Additional complications would arise were one to also consider a low-energy limit where the density of states is changing rapidly.

We found evidence that the introduction of a second space dimension has a slightly stronger effect on integrability than the introduction of the NNN coupling. In the NNN coupling study we saw no special behavior near $J_2/J = 0.24$ other than a resistance to level repulsion. It is perhaps not surprising that a qualitative change in the ground state does not affect the level statistics of the bulk of the states. On the other hand at non-negligible temperatures these higher-energy states would be important. Indeed the characteristic linear in temperature resistivity of the normal state of high-temperature superconductors persists up to $T > 500$ K. But we are a long way from formulating transport theory in terms of the random matrix approach. One must go far beyond simple level statistics in order to consider the response functions of an interacting fermion system.

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