Quantum Chaos in Spin-Fermion Models

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The full spectrum of a single hole in a quantum antiferromagnetic background (t-J_z-$J_\perp$ model) is obtained by complete exact diagonalization of small two-dimensional clusters. Various statistical properties of the spectrum are investigated. On a very wide range of the parameters the level-spacing distribution follows a Gaussian-orthogonal-ensemble Wigner law characteristic of chaotic spectra. At small separation, the spectral rigidity follows the universal behavior described by random-matrix theory and presents deviations at higher energies. We argue that quantum chaos is a generic feature of complex (i.e., nonintegrable) strongly correlated fermion systems.

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A large theoretical effort is currently being undertaken to achieve a better understanding of strongly correlated fermionic models in two dimensions (2D). The main motivation is the experimental realization of such systems in the high-T_c copper oxide superconductors. Although superconductivity in purely repulsive fermionic models remains the main issue, a large number of researches have been devoted to the understanding of the antiferromagnetic and metallic phases. The simplest (but still very complex) problem is the behavior of a single hole in an antiferromagnetic background. As we shall see later on, as far as statistical properties of the spectrum are concerned, this limit is expected to contain many generic features of strongly correlated systems.

In a pioneering work, Brinkman and Rice [1] introduced the retraceable path approximation to calculate the spectral density of a single hole moving in a classical Néel background. In order to preserve the antiferromagnetic order the hole, in first approximation, has to retrace its path. This mechanism leads to a large incoherent background in the single-hole spectral density. Later analytic work based on the Born approximation [2] or on exact diagonalization methods [3,4] showed that the incoherent nature of the hole spectral function (at sufficiently large energy) subsists when spin fluctuations are included. These studies also revealed the presence of elementary *low-energy* quasiparticle (δ-function) excitations (see also Ref. [5]). Very recently, the existence of the coherent band was confirmed by a finite-size scaling analysis [6]. However, apart from a narrow low-energy range, the many-body excitations cannot in general be described as a simple combination of elementary excitations. In this Letter, it is our purpose to study these excitations, i.e., to calculate the complete spectrum of the Hamiltonian, and investigate some of its statistical properties.

The study of spectral statistics in complicated systems has been initiated by Wigner, Dyson, Mehta, and others to describe the spectra of nuclei [7–9]. These authors describe the statistical properties of matrix Hamiltonians, with a Gaussian distribution of the elements around a zero average. A remarkable feature of the random-matrix theory (RMT) is that the distribution of levels depends only on the symmetry of the Hamiltonian. In particular, if the Hamiltonian is invariant under time-reversal symmetry, the statistical ensemble of matrices is invariant under orthogonal transformations and is called the Gaussian orthogonal ensemble (GOE). This RMT has been applied to a variety of very different physical situations in nuclear, atomic, and molecular physics [10,11]. The relevance of RMT to describe spectra of electronic systems was first pointed out by Gorkov and Eliashberg [12] and applied to disordered noninteracting electronic systems [13]. In the present case, the complexity results not from disorder but from the many-body nature of the Hamiltonian. In this paper, we show that a simple model of correlated electrons exhibits features characteristic of chaotic spectra well described by RMT.

The generic Hamiltonian in standard notations reads

$$\mathcal{H}=J_z\sum_{\mathbf{i},\epsilon}S^z_{\mathbf{i}}S^z_{\mathbf{i}+\epsilon}+\frac{1}{2}J_\perp\sum_{\mathbf{i},\epsilon}(S_{\mathbf{i}}^{+}S_{\mathbf{i}+\epsilon}^{-}+S_{\mathbf{i}}^{-}S_{\mathbf{i}+\epsilon}^{+})-t\sum_{\mathbf{i},\epsilon,\sigma}P_G[c^{\dagger}_{\mathbf{i},\sigma}c_{\mathbf{i}+\epsilon,\sigma}\exp(i\epsilon\cdot\kappa)+c^{\dagger}_{\mathbf{i}+\epsilon,\sigma}c_{\mathbf{i},\sigma}\exp(-i\epsilon\cdot\kappa)]P_G\,. \quad (1)$$

P_G is the Gutzwiller projector which enforces the constraint of no doubly occupied site. We have explicitly separated the diagonal (J_z) and the transverse parts ($J_\perp$) of the antiferromagnetic exchange coupling between neighboring sites $\mathbf{i}$ and $\mathbf{i}+\epsilon$, with $\epsilon=\mathbf{x}$ or $\mathbf{y}$. The Hamiltonian is defined on 2D $\sqrt{N}\times\sqrt{N}$ clusters defined on a torus ($N=16$ and 18 sites) and we assume arbitrary twists κ in the boundary conditions [14] ($\kappa=0$ corresponds to periodic boundary conditions, i.e., no twist). The twist κ_α in the α direction can alternatively be viewed as a magnetic flux penetrating one of the torus' hole.

It is important to notice that only a few group symmetries are left in the generic model (1). Trivially the particle

number is conserved. The Hamiltonian is also invariant under spin rotation around the z axis and under discrete translations. Hence, the Hamiltonian can be diagonalized in every sector of $S_z^{\rm tot}$ and of the total momentum $\mathbf{K}_p$. In fact, most of the results we report in this paper are generic and do not depend on the symmetry sector considered as long as one can totally separate it from the others [15]. Practically we shall consider the case of a single hole and $S_z^{\rm tot}=\frac{1}{2}$ in order to have the largest Hilbert space. Only in very specific cases, additional symmetries remain: (i) If $J_\perp=J_z=J$, (1) becomes isotropic in spin space (i.e., spin rotationally invariant). Since separating the various spin sectors is a difficult task we have left this problem for future work [16]. (ii) If $\kappa_\alpha=0$ ($\alpha=x$ or y) or $\kappa_x=\kappa_y$ some symmetries of the 2D square lattice are preserved (e.g., the 90° rotation around a site). The choice of arbitrary twists $\kappa_x\neq\kappa_y$ enables us to suppress the degeneracies due to these symmetries. Note that the $\sqrt{18}\times\sqrt{18}$ cluster [of translation vectors $\mathbf{T}_\gamma=(3,\pm 3)$, $\gamma=1,2$] is tilted by 45° with respect to the crystal axes.

Since the size $\mathcal{N}$ of the Hilbert space grows exponentially with the system size N, we have restricted our analysis to $N=16$ and 18 sites. By using $S_z^{\rm tot}$ (chosen as $\frac{1}{2}$) and translation symmetries we can already reduce $\mathcal{H}$ to $\mathcal{N}\times\mathcal{N}$ blocks with respectively $\mathcal{N}=6435$ and $\mathcal{N}=24310$ for 16 and 18 sites. The full spectrum (i.e., the $\mathcal{N}$ eigenvalues) is calculated in two steps: (i) A Jacobi matrix (tridiagonal) is generated by applying recursively the Hamiltonian on an arbitrary initial (nonsymmetric) spin-hole configuration, and (ii) a bisection method is used to further diagonalize the Jacobi matrix. To get all the eigenvalues of the original matrix, it appears that, in step (i), it is often necessary to perform more than $\mathcal{N}$ iterations (typically $\sim 2\mathcal{N}$). The irrelevant eigenvalues are then eliminated by standard methods [17]. Note that in this approach, the CPU time grows like $\mathcal{N}^2$ contrary to the $\mathcal{N}\ln\mathcal{N}$ scaling in the standard Lanczos algorithm procedure restricted to the obtaining of only the *lowest* excited levels [3,4,6]. The complete diagonalization of the largest system ($N=18$ in the case $J_\perp=0$) required 60000 iterations and ~ 2 h of CPU on a Cray-2 computer. By the two-step procedure described above one could in principle get the spectra $\{E_\mu(\mathbf{K}_p,S_z^{\rm tot},\boldsymbol{\kappa})\}$ ($\mu=1,\ldots,\mathcal{N}$, $p=1,\ldots,N$) in all the symmetry sectors. However, most of the results derived in this paper do not depend on the quantum numbers $\{\mathbf{K}_p,S_z^{\rm tot}\}$ (as long as the system is not spin polarized) or on the flux variable $\boldsymbol{\kappa}$ so that we can restrict ourselves to any particular value.

The density of states $N_{\rm tot}(E)=\sum_\mu\delta(E-E_\mu)$ is shown in Fig. 1 and is almost flat over a wide energy range. The average level spacing is $\propto N/\mathcal{N}$ (except at the edges of the spectrum). At this stage, it is important to discuss briefly the differences between $N_{\rm tot}$ and well-known spectral densities of the form $A(\omega)=\sum_\mu|A_{0\mu}|^2\delta(\omega-E_\mu+E_0)$ (extensively studied, e.g., in numerical calculations) where the weighting factor $|A_{0\mu}|^2$ is simply the

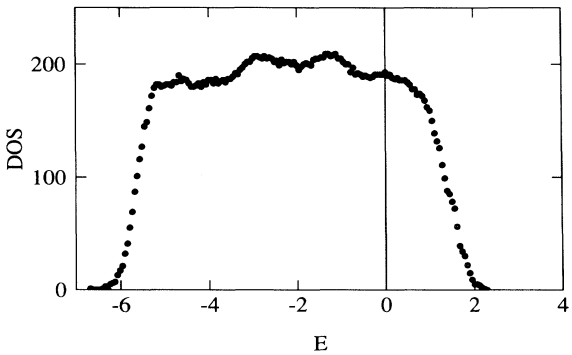

FIG. 1. Density of states of the t-J_z model for $N=18$ and $J_z=0.25$. The horizontal axis is labeled in terms of the *total* energy ($\propto N$).

square of the matrix element $\langle\Psi_0|O|\Psi_\mu\rangle$ where O is some operator of physical interest. In general, O generates only low-energy excitations $|\Psi_\mu\rangle$ above the ground state $|\Psi_0\rangle$ (like particle-hole or spin-wave excitations) so that $A(\omega)$ is exponentially suppressed for excitation energies ω ($=E-E_0$) larger than some characteristic energy scale (typically t or J) whereas the full spectrum (measured from the ground-state energy) is not bounded (when $N\to\infty$).

We have first studied the spacing distribution $P(s)$ between consecutive levels. As a standard procedure, we have first "unfolded" the spectrum E_μ by the transformation $x_\mu=N_{\rm av}(E_\mu)$ where $N_{\rm av}$ is the smoothed integrated density of states [11], so that the unfolded spectrum has a constant density of states. In addition, we have eliminated 1000 eigenvalues on each side of the spectrum. The result is shown in Fig. 2 for $N=18$, $J_z=0.25$, and $J_\perp=0$. It is very well fitted by the Wigner surmise for the GOE [9]:

$$P(s)=\tfrac{1}{2}\pi s\exp(-\tfrac{1}{4}\pi s^2)\,, \qquad (2)$$

where s is the distance between levels in units of the average interlevel distance. The repulsion between levels [$P(s)\to 0$ when $s\to 0$] is the signature of a chaotic behavior for the underlying classical system. It is of impor-

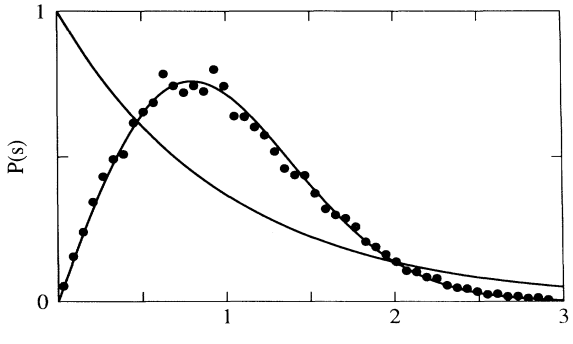

FIG. 2. Level spacing distribution $P(s)$ in the t-J_z model for $N=18$ and $J_z=0.25$. Ideal GOE and Poisson distributions are shown as full lines.

tance to notice that the GOE fits our results even in the presence of a twist in the boundary conditions. *A priori* this twist breaks time-reversal symmetry: Under $T:\kappa \rightarrow -\kappa$ the Hamiltonian (1) is no longer invariant but rather transforms into its complex conjugate. As a result, one could expect to observe statistical properties characteristic of the Gaussian unitary ensemble (GUE) relevant to the case of non-time-reversal invariant systems.

However, for any symmetry $\mathcal{G}$ of the point group (C_{4v}) of the cluster we have, $E_\mu(\mathcal{G}(\mathbf{K}_p), S_z^{\rm tot}, \mathcal{G}(\kappa)) = E_\mu(\mathbf{K}_p, S_z^{\rm tot}, \kappa)$ [7]. Hence it becomes clear that under time reversal the spectra corresponding to $\mathbf{K}_p$ and $-\mathbf{K}_p$ are simply interchanged. The Hamiltonian is then invariant under the product $T \times I$ where I is the inversion in real space, $I:\mathbf{R} \rightarrow -\mathbf{R}$ (the origin is arbitrary). This invariance under such an "antiunitary" transformation leads to GOE spectral fluctuations rather than those of the GUE [18].

Although our investigation was restricted to a very special model of strongly correlated fermions we speculate that level repulsion is in fact a general feature of most interacting quantum systems in solid-state physics (e.g., it should also occur in purely spin systems). Certainly, such a general phenomenon is expected to have implications for many physical properties which remain to be investigated. On the other hand, only a limited number of integrable models—like solvable one-dimensional models (e.g., one-dimensional Heisenberg or Hubbard model [19])—probably still show a Poissonian distribution with absence of level repulsion.

We also notice that the study of $P(s)$ alone can both (i) give hints whether the quantum model is solvable and (ii) suggest whether chaos occurs in the classical counterpart of the quantum model. Indeed, the Poisson and GOE spectra are associated with integrable and chaotic classical underlying models, respectively. While the test of RMT has been used on systems with small numbers of degrees of freedom, our study suggests that it may be extended to models of statistical mechanics. Let us mention that in the particular case studied here one can easily define some classical limit $S \rightarrow \infty$ (at least when $t=0$) in which the classical spins live on the sphere.

An interesting way to investigate the nature of the spectral statistics is to plot the quantity $\Sigma^2(E)$ which measures the fluctuation of the number of levels $N(E)$ in a strip of width E, $\Sigma^2(E) = \langle N^2(E)\rangle - \langle N(E)\rangle^2$. Like for the calculation of $P(s)$, the average is done on the whole spectrum except 1000 levels on each side. The results are shown in Figs. 3(a)–3(d) for various parameters. At low energy, $\Sigma^2(E)$ follows very well the GOE behavior. Deviations appear at higher energy, which depend on the size of the sample and on the parameters of the problem. In particular, it is seen that when J_z increases from 0.25 [Fig. 3(a)] to 2 [Fig. 3(b)], $\Sigma^2(E)$ deviates more from the GOE behavior while $P(s)$ is still given by the Wigner surmise (2). Note that, in the extreme limit $J_z/t \rightarrow \infty$,

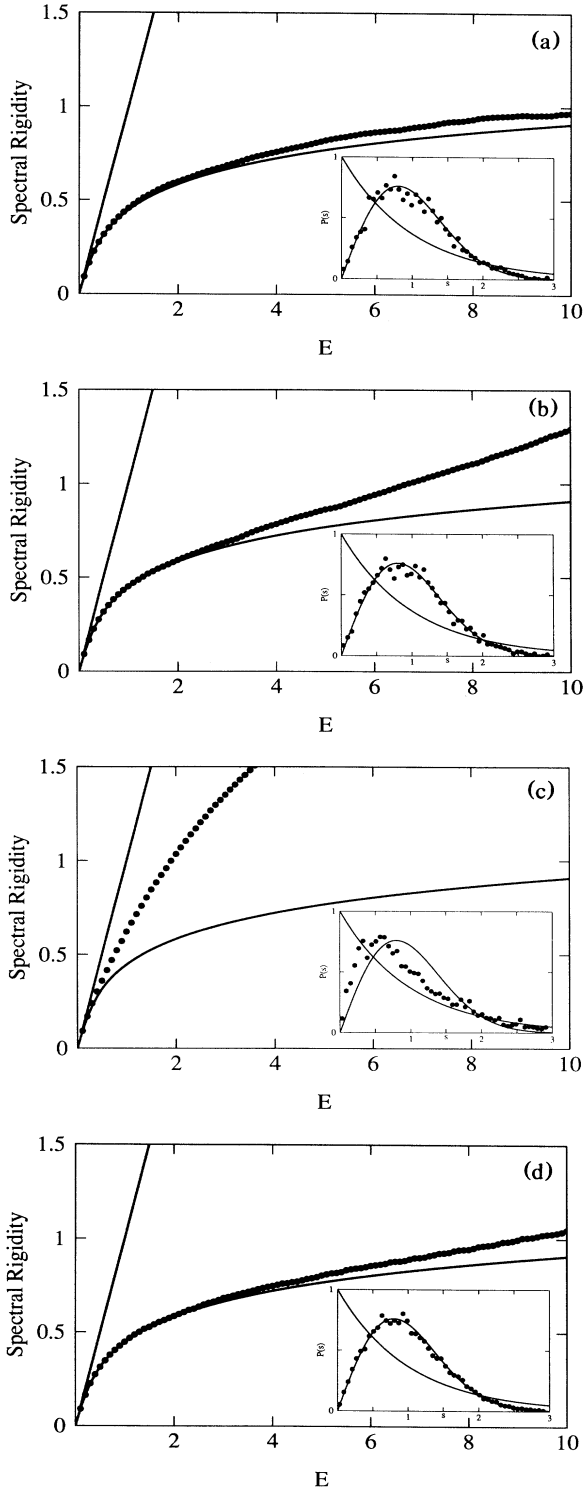

FIG. 3. Spectral rigidity Σ^2 vs energy. The linear and logarithmiclike solid curves correspond respectively to the ideal Poisson and GOE behaviors. (a) $N=16$, $J_z=0.25$, and $J_\perp=0$; (b) $N=16$, $J_z=2$, and $J_\perp=0$; (c) $N=16$, $J_z=0.25$, and $J_\perp/J_z=0.95$; (d) $N=18$, $J_z=0.25$, and $J_\perp=0$. Inset: Corresponding level-spacing distribution.

huge degeneracy appears and the spectrum is made of equally spaced levels that lead to delta functions at $s=1$ and $s=0$ in $P(s)$. As seen previously, a nonzero hopping t changes $P(s)$ drastically, although we do not know precisely where this crossover occurs. On the other hand, when $J_\perp$ increases [$=0.95$ in Fig. 3(c)], $P(s)$ deviates more and more from GOE and tends to become Poissonian. This tendency is confirmed by the behavior of $\Sigma^2(E)$. Indeed, for $J_\perp/J_z \to 1$ the spin rotational invariance is recovered and the total spin becomes a good quantum number. Since, practically, we do not separate the various spin sectors we start to mix several GOE spectra, and the statistics of the resulting spectrum becomes Poissonian as expected. However, it is very probable that the total spin being a good quantum number has no bearing on the level repulsion [20]. In other words, in each spin sector, the statistics would remain GOE. As seen from a direct comparison of Figs. 3(a) and 3(d) which correspond respectively to 16 and 18 sites and the same set of parameters, the spectral rigidity does not depend crucially on the system size. It is notable that an increase of the Hilbert space by a factor ~ 4 does not lead to any significant modification of the spectral rigidity.

We finish this Letter by briefly discussing the connections between this work and standard approaches to the problem of strongly correlated fermions. A central issue is whether or not the GOE statistics rules out a Fermi liquid description or more generally any perturbation expansion from a noninteracting limit. If *many-body* low-energy excitations can be built from renormalized elementary excitations (e.g., quasiparticles in Landau Fermi liquid theory, spin waves in quantum antiferromagnets) and if interactions between these excitations are neglected, one would expect the system to be in essence similar to a noninteracting or integrable model and hence to have a Poissonian statistics *at low energy*. On the other hand, recent numerical calculations [6] have confirmed the presence of a quasiparticle peak in the one-hole spectral function. Such features are rather general and are present in many dynamical correlation functions such as the spin structure factor (in that case, the spin-wave excitations play the role of the quasiparticle excitations). How does this reconcile with the GOE statistical property of the spectrum? There might be so far two possible explanations (which are not mutually exclusive): (i) First, the elementary excitations are expected only in a narrow energy range above the ground-state energy whereas the present study deals with the full spectrum with an exponentially large (compare to N) number of states at higher energies. (ii) Even at low energies, because of the interactions between elementary excitations, the problem does not reduce to a true noninteracting problem. Hence, our results do not rule out renormalized *low-energy* quasiparticle excitations but shows that a statistical description analogous to the RMT is appropriate at higher energies.

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