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The spectrum of the two-dimensional Hubbard model at low filling

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Abstract. – The entire energy spectrum is calculated numerically for the two-dimensional Hubbard model on square lattices with four electrons varying the interaction strength U in a wide range. Taking all symmetries explicitly into account a level statistical analysis is performed on this strongly correlated 2D system. The level spacing distribution and the number variance exhibit a random matrix (GOE) behavior for *all* positive values of U, the latter however only up to a medium energy scale $\lambda^* \approx 3$ independent of U.

The surprising discovery of high-temperature superconductivity in complicated cuprates containing planes of conducting electrons has renewed the interest in the study of two-dimensional strongly correlated electronic systems. One of the simplest models describing such systems is the Hubbard model [1], but in spite of its apparent simplicity this model turns out to be extremely difficult to fully understand (see, *e.g.*, the recent reviews ref. [2], [3]). This is mainly due to the lack of a small parameter which makes the use of well-established perturbative methods highly questionable. In this state of affairs the importance of performing numerical calculations of the spectrum for finite clusters has grown.

We study the spectrum of the two-dimensional Hubbard model using a random matrix analysis [4] of the spectral statistics thereby extending previous work on 1D systems [5]-[7] to 2D. For the 1D systems there is a growing evidence for the following fact concerning the distribution $P(s)$ of the energy level spacings s: if the system is integrable, *e.g.* by the Bethe ansatz, $P(s) = e^{-s}$ (the Poisson distribution as for the random diagonal matrix ensemble), while if it is non-integrable $P(s) = (s\pi/2)\exp[-s^2\pi/4]$ (the Wigner distribution as for the Gaussian Orthogonal Ensemble (GOE)). Our random matrix analysis is not restricted only to comprise $P(s)$ since several statistical processes with the same short-range correlations lead to that level spacing distribution. We, therefore, also study the number variance $\Sigma_2(\lambda)$ which includes long-range correlations [4].

The model. – In this paper we study the one-band Hubbard model containing nearest-neighbor hopping and on-site interaction:

$$\hat{H} = -t\hat{T} + U\hat{U} \equiv -t \sum_{\langle i,j\rangle,\sigma} \hat{c}^{\dagger}_{j\sigma}\hat{c}_{i\sigma} + U \sum_{i} \hat{n}_{i\uparrow}\hat{n}_{i\downarrow} \,. \tag{1}$$

We treat the case of two-dimensional $L \times L$ square lattices with periodic boundary conditions, and to investigate the low-filling properties of the model close to but not in the integrable dilute limit ($L \to \infty$) [8], we restrict ourselves to four electrons. We let L vary from 4 to 6 and obtain the filling factors 0.13, 0.08, and 0.06, respectively. The periodic boundary conditions lead to the largest possible space symmetry group, a feature essential to our study.

Group-theoretical and numerical analysis. – A careful group-theoretical analysis enables us to sort the states with respect to *all* known quantum numbers. This is not only a prerequisite for the analysis of the spectral statistics, but it also makes possible the numerical diagonalization of the Hubbard Hamiltonian on lattices as big as the 6×6 square lattice. We construct the symmetry projection operators corresponding to all known symmetries of the model and use them to project into symmetry-invariant subspaces of the full Hilbert space [9]. For our study it is essential to keep all symmetries in the model, rather than adding extra terms to $\hat{H}$ and sorting out the symmetries after diagonalization as is commonly done. This makes the group-theoretical analysis more complex, but it leads to larger reductions, and yields more precise numerical results. To further facilitate the calculation of spectra for arbitrary values of U/t, we calculate and store matrix elements of the operators $\hat{T}$ and $\hat{U}$ rather than of $\hat{H}$. Then for any given value of U/t the spectrum is calculated by standard numerical diagonalization of $-t\hat{T} + U\hat{U}$ [10].

The first symmetry we consider is the space group G_L of the lattice. It consists of all permutations g mapping any neighboring sites i and j onto neighboring sites $g(i)$ and $g(j)$. In a straightforward manner an operator $\hat{g}$ in the Hilbert space can be associated to each element g of G_L thus forming a group $\hat{G}_L$ of operators. For any lattice size G_L has been analyzed in detail in ref. [11]. It was found that $G_L = D_L \otimes D_L \circledS Z_2$, where D_L is the dihedral group of index L, and each irreducible representation was related to the momentum of the eigenstates. However, this result is *not* valid for the special case $L = 4$. In this work we use the correct G_4 which turns out to be isomorphic with the group of transformations of the 4D hypercube [10], [12]. To deal with the space symmetry, we employ the projection operators $\hat{\mathcal{P}}^{(R)}_k$ of row k in representation R of G_L having the usual form $\frac{l_R}{h}\sum_g \Gamma^{(R)*}_{kk}(g)\,\hat{g}$ [9].

Next is the $SU(2)$ spin symmetry. $\hat{H}$ commutes with the total spin $\hat{\mathbf{S}}$ and with the corresponding raising and lowering operators $\hat{S}_+$ and $\hat{S}_-$, so without loss of generality we work in the $\hat{\mathbf{S}}_z = 0$ sector; the spectra of the other sectors are trivially constructed using $\hat{S}_+$ and $\hat{S}_-$. Moreover, $\hat{\mathbf{S}}$ commutes with all operators of $\hat{G}_L$, and the combination of the two groups is a direct product. The spin symmetry of four-electron states is dealt with through the projections $\hat{\mathcal{P}}^{(S)}|a\uparrow, b\uparrow, c\downarrow, d\downarrow\rangle$ having the form $\sum_\pi \alpha^\pi_{abcd}|\pi_a\uparrow, \pi_b\uparrow, \pi_c\downarrow, \pi_c\downarrow\rangle$, where π is a permutation of the sites *abcd* [10].

The last of the known symmetries is the $SU(2)$ pseudospin symmetry [13]. It exists only for bipartite lattices, which for periodic square lattices demands L to be even. The generators of the $SU(2)$ pseudospin symmetry are $\hat{J}_- = \sum_i (-1)^i \hat{c}_{i\uparrow}\hat{c}_{i\downarrow}$, $\hat{J}_+ = \hat{J}^{\dagger}_-$, and $\hat{J}_z = \frac{1}{2}(\hat{N} - L^2)$, where $\hat{N}$ is the electron number operator. The pseudospin $\hat{J}$ commutes with $\hat{H}$ as well as with all $\hat{g} \in \hat{G}_L$ and $\hat{S}$. For $\hat{J}$ we find the projection $\hat{\mathcal{P}}^{(J)}|a\uparrow, b\uparrow, c\downarrow, d\downarrow\rangle$ to be of the form $\sum_\pi \beta^\pi_{abcd}|\pi_a\uparrow, \pi_b\uparrow, \pi_c\downarrow, \pi_c\downarrow\rangle$, where $\pi_a\pi_b\pi_c\pi_d$ are sites related to *abcd* by the pair hopping operator $\hat{J}_+\hat{J}_- + \hat{J}^2_z - \hat{J}_z$ [10].

A detailed analysis shows that combining the spin and the pseudospin symmetries yields an $SO(4)$ symmetry rather than an $SU(2) \otimes SU(2)$ symmetry [14]; however, the projection operators still form direct products. The full symmetry group for even L is $\mathcal{G} = G_L \otimes SO(4)$, and in addition to the principal energy quantum number n the states are labeled with the three quantum numbers R, S, and J corresponding to the total projection operator $\hat{\mathcal{P}}_k^{(R)} \otimes \hat{\mathcal{P}}^{(S)} \otimes \hat{\mathcal{P}}^{(J)}$. For L odd $\mathcal{G} = G_L \otimes SU(2)$, and only R and S are defined. In row 2 and 3 of table I we show the dimension of the total Hilbert space and the much smaller dimension of the largest symmetry-invariant subspace found by the group-theoretical analysis.

Finally, after numerical diagonalization of $\hat{H}$ in each invariant subspace, simultaneous eigenstates of $\hat{H}$ and $\hat{U}$ are discarded from the level statistical analysis since such states are unaffected by the interaction. We note that all states with maximal spin ($S = 2$) are among these states. In row 4 of table I we show that no degeneracy remains after projecting into the symmetry-invariant subspaces and discarding U-independent states. In the following three rows of table I we list for completeness the number of U-independent states (the $\hat{U}$-eigenstates) for each of the three possible $\hat{U}$-eigenvalues λ_U. Note that among these states some degeneracy remains even after the symmetry projection. The main result of this section is that no degeneracy remains among the U-dependent states within each invariant subspace; and consequently we are in a position to perform the level statistical analysis.

TABLE I. – *For $L = 4, 5,$ and 6 the dimension $\dim(\mathcal{H})$ of the total unreduced Hilbert space and the dimension $\dim(\mathcal{I})$ of the largest symmetry-invariant subspace are shown. Furthermore, in the row U-dep we show the number of U-dependent energy eigenstates while in the rows λ_U we show the number of U-independent energy eigenstates also being eigenstates of $\hat{U}$ with eigenvalue λ_U. The columns non-d/deg refer to the number of (non-)degenerate states within the symmetry-invariant subspaces.*

	$L = 4$		$L = 5$		$L = 6$	
$\dim(\mathcal{H})$	14400		90000		396900	
$\dim(\mathcal{I})$	146		1794		5490	
	non-d	deg	non-d	deg	non-d	deg
U-dep	8641	0	73639	0	280042	0
$\lambda_U = 0$	155	5389	860	15501	376	116167
$\lambda_U = 1$	176	38	0	0	99	207
$\lambda_U = 2$	1	0	0	0	1	8

Level statistics. – The first step in the level statistical analysis is the "unfolding" of the spectrum in order to transform the energies E_n into "reduced energies" ε_n of constant density. This amounts to carefully computing an average cumulative density of states $N_{\mathrm{av}}(E)$ from the actual cumulative density of states [4]. In the limits $U \ll W$ and $U \gg W$, W being the band width, large gaps appear in the spectrum. For small U these gaps are due to the finite size of the lattice while for large U they are due to the formation of well-separated Hubbard bands. To unfold the spectrum we employ the method of substituting the delta-function peaks of the density of states with Gaussian peaks of finite width σ. For each subband q separated by the

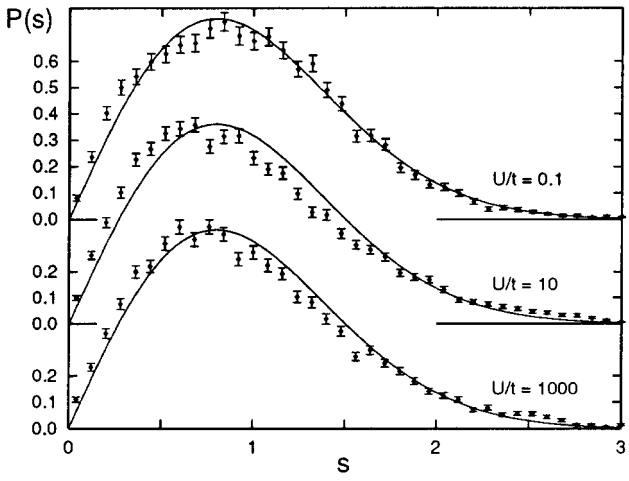

Fig. 1. – The probability distribution $P(s)$ of the level spacings s in the unfolded 5×5 Hubbard model spectrum averaged over all symmetry sectors in the three cases of small, medium, and large interaction strength U/t. The full line is the Wigner distribution found for GOE random matrices.

gaps we choose a Gaussian width of the form $\sigma_q = C\Delta_q$, where C is a constant and Δ_q is the average level spacing within the subband. We find that the level spacing distribution $P(s)$ is fairly independent of the actual value of C whereas the number variance $\Sigma_2(\lambda)$ depends on the choice of C. We, therefore, select that value of C which leads to the best fit of $\Sigma_2(\lambda)$ to the corresponding GOE curve. This unfolding procedure was tested for an ensemble of GOE random matrices and it was found to agree very well with the unfolding based on the semi-circular density of states.

To study the statistical properties of the spectrum at small energy scales we calculate $P(s)$. The result for three different values of U/t spanning four orders of magnitude is shown in fig. 1. In all three cases $P(s)$ is close to the Wigner distribution; it possesses a pronounced linear level repulsion for small s, a peak near $s = 1$ signaling spectral rigidity, and a Gaussian tail. At this level of the analysis we find no significant difference between RMT and the spectrum of the Hubbard model. We, therefore, proceed to study the statistical properties of the spectrum on larger energy scales and higher correlation choosing to focus on the number variance $\Sigma_2(\lambda)$ defined as the variance of the number $\nu(\varepsilon, \lambda)$ of unfolded energy levels in intervals of length λ around the unfolded energy ε [4]:

$$\Sigma_2(\lambda) = \left\langle (\nu(\varepsilon, \lambda) - \lambda)^2 \right\rangle_\varepsilon \ . \tag{2}$$

The brackets denote an averaging over ε. Figure 2 shows $\Sigma_2(\lambda)$ of the Hubbard model for $U/t = 0.1$, 10, and 1000 averaged over all symmetry sectors. When λ is small the rigidity of the Hubbard spectrum is very close to that of the GOE random matrices, while for larger λ a saturation sets in. For all three values of U/t we find the critical value λ^* where the departure from GOE sets in to be roughly 3. We note that this behavior is qualitatively different from that found recently in a system consisting of two intacting particles in a disordered environment in 1D. In the latter system $\Sigma_2(\lambda)$ were found to break away from the GOE curve at $\lambda \approx 1$ with a power law *increase* [15]. We can conclude that only up to a medium energy scale $\lambda^* \approx 3$ a true RMT behavior of the Hubbard model is found. This conclusion also holds for the $L = 4$ and 6 lattices.

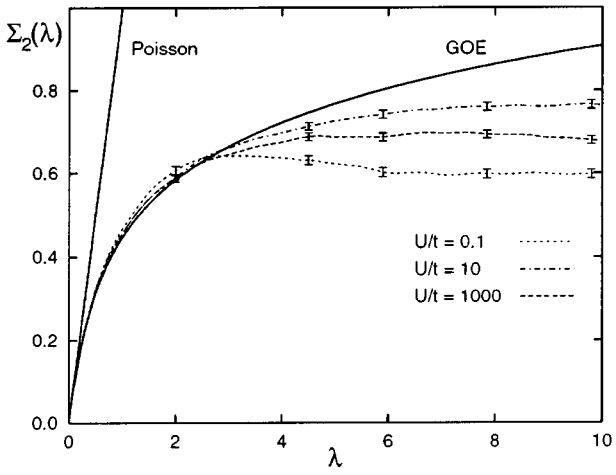

Fig. 2. – The number variance $\Sigma_2(\lambda)$ of the unfolded 5×5 Hubbard model spectrum for $U/t = 0.1$, 10, and 1000 averaged over all symmetry sectors and compared to the results of the random diagonal matrix ensemble (Poisson) and the random full matrix ensemble (GOE).

Conclusion and discussion. – The exact spectrum of the 2D Hubbard model at low filling has been calculated numerically by projecting the Hamiltonian into invariant subspaces of all the known symmetries for a wide range of U/t and for three different square lattices.

For the first time the commonly used statistical analysis of random matrix spectra has been applied to a strongly correlated 2D fermion system. The level spacing distribution $P(s)$ shows an excellent agreement with RMT. However, the number variance $\Sigma_2(\lambda)$ agrees only with RMT up to the U/t-independent medium-sized energy scale $\lambda^* \approx 3$. Beyond λ^* a saturation sets in, an effect to be studied further in forthcoming work. We stress that the GOE-like behavior at small energy scales has been found not only for *all* finite values of U/t including values close to the integrable $U/t = 0$ and $U/t = \infty$ limits, but also for filling factors as low as 0.06 close to the integrable dilute limit ($L \to \infty$). This emphasizes the non-perturbative nature of the model revealed by our analysis: even the smallest deviation from the integrable limits leads to spectral statistics usually associated with non-integrability and quantum chaos.

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