The Spectrum of the two dimensional Hubbard model at low filling

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Using group theoretical and numerical methods we have calculated the exact energy spectrum of the two-dimensional Hubbard model on square lattices with four electrons for a wide range of the interaction strength. All known symmetries, i.e. the full space group symmetry, the SU(2) spin symmetry, and, in case of a bipartite lattice, the SU(2) pseudospin symmetry, have been taken explicitly into account. But, quite remarkably, a large amount of residual degeneracies remains giving strong evidence for the existence of a yet unknown symmetry. The level spacing distribution and the spectral rigidity are found to be in close to but not exact agreement with random matrix theory. In contrast, the level velocity correlation function presents an unexpected exponential decay qualitatively different from random matrix behavior.

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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 interacting 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 review by E. Dagotto 2). This is mainly due to the lack of a small parameter which makes the use of well established perturbative methods in condensed matter theory highly questionable. In this state of affairs the importance of performing numerical calculations of the spectrum for finite clusters has grown.

On the other hand the concept of level statistics has proven itself to be a useful tool in the understanding of non-perturbative many-body quantum systems. Originally applied to models in nuclear physics 3 the method consists of describing some spectral properties of the Hamiltonian by those of a well suited ensemble of random matrices. The ensemble of random matrices to be chosen depends on the physical system under consideration. For example a system which can be solved by the Bethe Ansatz displays the same distribution, \( P(s) \), of the energy level spacings \( s \) as an ensemble of random diagonal matrices, i.e. a Poisson distribution \( P(s) = e^{-s} \). In contrast \( P(s) \) for non-integrable time reversal symmetric systems has been found empirically to be the same as that for the Gaussian Orthogonal Ensemble (GOE), i.e. a Wigner distribution \( P(s) = (s\pi/2)\exp(-s^2\pi/4) \).

The appearance of a Wigner distribution is interpreted in terms of level repulsion: states belonging to the same symmetry class repel each other. This gives a connection between quantum chaos and the level distribution.

In this letter we extend the level statistical analysis of quantum Hamiltonians 3,4,5 to include the two dimensional Hubbard model with four electrons (low filling) as a function of the coupling strength \( U/t \) to be defined below. Our study is not restricted only to comprise \( P(s) \); the spectral rigidity \( \Delta_3(\lambda) \) is also investigated in detail as well as the level velocity correlation \( c(x) \), a quantity related to the deformation of the spectrum when \( x \sim U/t \) is varied. A careful group theoretical analysis enables us to sort the states with respect to all known quantum numbers and makes possible the numerical diagonalization of the Hubbard Hamiltonian on lattices as big as the 6 x 6 square lattice. Residual degeneracies in the resulting spectra constitute the first numerical evidence of the existence of a new unknown symmetry of the Hubbard model. Further traces of this new symmetry are seen as small deviations from the expected random matrix behavior of \( P(s) \) and \( \Delta_3(\lambda) \).

Group theoretical and numerical analysis. Throughout this letter we study the one–band Hubbard model containing nearest–neighbor hopping and on–site interaction:

\[
\hat{H} = -t\hat{T} + U\hat{V} \equiv -t \sum_{(i,j),\sigma} \hat{c}^\dagger_{j\sigma}\hat{c}_{i\sigma} + U \sum_i \hat{n}_i \hat{n}_i .
\] (1)

We treat the case of a two dimensional \( L \times L \) square lattice with periodic boundary conditions. To investigate the low filling properties of the model we restrict ourself to four electrons. We vary \( L \) from 3 to 6 and obtain the filling factors 0.22, 0.13, 0.08, and 0.06 respectively. To achieve the a priori maximal reduction of the problem 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 \( \mathcal{H} \). 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 it yields more precise numerical results. To facilitate further the calculation of spectra for arbitrary values of \( U/t \) we calculate and store matrix elements of the operators \( \hat{T} \) and \( \hat{V} \) rather than of \( \hat{H} \). Then for any given value of \( U/t \) the spectrum \( E(U/t) \) as well as the derivative \( \partial E/\partial(U/t) \) is calculated by straightforward diagonalization of \(-t\hat{T} + U\hat{V} \) 3.
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 $g(j)$. To each element $g$ of $G_L$ an operator $\hat{g}$ in the Hilbert space can be associated in a straightforward manner forming a group $\hat{G}_L$ of operators. For any lattice size $G_L$ has been analyzed in detail by Fanò, Ortolani, and Parola [1] and found to be $D_L \otimes D_L \otimes Z_2$, where $D_L$ is the usual dihedral group of index $L$. However, this result is not valid for the special case $L = 4$, where the spatial group is three times larger. In this work we use the correct $G_4$ [8]. To deal with the space symmetry we employ the projection operators $\hat{P}^{(R)}_k$ of row $k$ in representation $R$ of $G_L$, having the usual form $\frac{1}{4\pi} \sum_g \Gamma^{(R)*}_{kk}(g) \hat{g}$ [8].

Next is the SU(2) spin symmetry. Since $H$ commutes with the total spin $\hat{S}$ and with the corresponding raising and lowering operators $\hat{S}_+$ and $\hat{S}_-$, we work in the $S_z = 0$ sector, i.e. with two up spins and two down spins. Moreover, $\hat{S}$ commutes with all operators of $G_L$, and the combination of the two groups is a direct product. The spin symmetry of four-electron states is dealt with through the projections $\hat{P}^{(S)}(a \uparrow, b \uparrow, c \downarrow, d \downarrow)$ having the form $\sum_r \alpha_{abcd} \pi_r \uparrow, \pi_b \uparrow, \pi_c \downarrow, \pi_d \downarrow$, where $\pi$ is a permutation of the sites $abcd$ [4].

The last of the known symmetries is the SU(2) pseudospin symmetry. This symmetry of dynamical origin based on the $\eta$-paring mechanism was discovered recently [4]. It exists only for bipartite lattices, for which periodic square lattices demands $L$ to be even. The generators of the SU(2) pseudospin symmetry are:

$$\hat{J}_- = \sum_i (-1)^i \hat{c}_i \hat{c}_i^\dagger, \quad \hat{J}_+ = \hat{J}_x^\dagger, \quad \hat{J}_z = \frac{1}{2}(\hat{N} - L^2),$$

where $\hat{N}$ is the electron number operator. The pseudospin $\hat{J}$ commutes with $H$ as well as with all $\hat{g} \in \hat{G}_L$ and $\hat{S}$. For $J$ we find the projection $\hat{P}^{(J)}(u \uparrow, v \uparrow, c \downarrow, d \downarrow)$ to be of the form $\sum_{\pi} \beta_{abcd} \pi_r \uparrow, \pi_b \uparrow, \pi_c \downarrow, \pi_d \downarrow$, where $\alpha_{\pi_0 \pi_1 \pi_2 \pi_3}$ are sites related to $abcd$ by the pair hopping operator $\hat{J}_x \hat{J}_x + \hat{J}_x^2 - \hat{J}_z^2$ [3].

A detailed analysis shows that combining the spin and the pseudospin symmetries yields a SO(4) symmetry rather than a SU(2) $\otimes$ SU(2) symmetry [11], however, the projection operators still form direct products. The full symmetry group for even $L$ is $G = G_L \otimes SO(4)$, 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 $\hat{P}^{(R)}_k \otimes \hat{P}^{(S)}_k \otimes \hat{P}^{(J)}_k$. For $L$ odd $G = G_L \otimes SU(2)$, 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.

A new symmetry. The most remarkable fact revealed by Table I is the large amount of residual degeneracies present after sorting the spectrum according to all known symmetries. We note that states with the maximal spin $S = 2$ contain no doubly occupied sites. They are thus independent of $U$ and are consequently excluded from our study. States with $S = 1$ $(S = 0)$ can accommodate up to one (two) doubly occupied site(s) and in general they are therefore expected to depend on $U/t$. Nevertheless, it turns out that there exist states with $S = 0$ and $S = 1$ which are independent of $U$. This is the first evidence that an additional symmetry exists in the problem. Much stronger evidence comes from the existence of degeneracies remaining after excluding accidental inter-representational degeneracies as well as the trivial $l_R$-fold degeneracy of the $l_R$ rows in a given representation of the space group. This result is summarized in row 4 to 7 of Table I showing the total number of $U$-(in)dependent and (non-)degenerated states. It is seen that almost all the residual degenerated states are $U$-independent. In fact only for even $L$ we found a few $U$-dependent degenerated states, and they all belong to invariant subspaces with a dimension smaller than 7. We stress that finding the residual degeneracies was only possible because of the relatively small size of the symmetry invariant subspaces enabling us to employ the standard iterative diagonalization techniques [8]. It is extremely difficult to find degeneracies using the Lanczos method.

Level statistics. Based on Table I we conjecture that the new symmetry is related to the $U$-independent states. We therefore exclude all such states from our treatment. The results we show in the figures below are obtained with $L = 5$ because this is the largest lattice for which all states have been computed. The results for other values of $L$ are similar.

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’ $\varepsilon_n$ of constant density. This amounts to carefully computing the average cumula-

| $L$ | 3 | 4 | 5 | 6 |
|-----|---|---|---|---|
| $\text{Dim}(H)$ | 1,296 | 14,000 | 90,000 | 396,000 |
| $\text{Dim}(L)$ | 38 | 146 | 1,794 | 5,490 |
| $S=0.1$ | deg. $U$-indep. | 0 | 3,662 | 3,139 | *13,120 |
| $S=0.1$ | deg. $U$-dep. | 0 | 38 | 0 | *19 |
| $S=0.1$ | non-deg. $U$-indep. | 9 | 62 | 572 | *64 |
| $S=0.1$ | non-deg. $U$-dep. | 1161 | 8,818 | 73,639 | *50,418 |
| $S=2$ | $U$-indep. | 126 | 1,820 | 12,650 | 58,905 |

TABLE I. For $L = 3, 4, 5,$ and 6 are shown the dimension $\text{Dim}(H)$ of the total unreduced Hilbert space, the dimension $\text{Dim}(L)$ of the largest symmetry invariant subspace, and the number of degenerated and non-degenerated levels dependent or independent of $U/t$ for the three values of the total spin $S$ after taken all known symmetries into account. The numbers marked by * in the $L = 6$ column covers only 36 out of 130 representations (18% of the 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 six 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. However, the statistics are good enough to note a significant discrepancy, and in fact on a 99.99% confidence level a $\chi^2$ test leads to a rejection of the hypothesis that $P(s)$ is Wigner distributed for any of the three values of $U/t$. The level repulsion is not as strong as expected from a GOE spectrum. We interpret this as another trace of the remaining symmetry, and we speculate that if we could sort the states according to the new symmetry, then the level repulsion would be stronger and $P(s)$ would be closer to the Wigner distribution.

It should be noted, though, that the new symmetry does not mix the symmetry classes very much, so in a sense the known symmetries nearly sort the spectrum perfectly, and in fact for some individual representations for $L = 6$ a $\chi^2$ test does not lead to rejection.

The brackets denote an averaging over $\epsilon_0$. Fig. 2 shows $\Delta_3(\lambda)$ of one specific symmetry sector for five different values of the interaction strength $U/t$ ranging from 1, close to the integrable non–interacting case, to 20, well into the strongly interacting regime. When $\lambda$ is small the rigidity of the Hubbard spectrum is very close to that of the GOE random matrices, while for larger $\lambda$ the spectra becomes less rigid; i.e. on a large energy scale the levels become uncorrelated, even though adjacent levels are strongly correlated. The reason for this behavior is that the strong degeneracies existing at $U/t = 0$ is slowly lifted as $U/t$ is increased. For small values of $U/t$ levels within each degeneracy band interact. Hence for small $\lambda$ only properly randomized levels are sampled by $\Delta_3(\lambda)$.

If $\lambda$ is larger than the typical width of the bands, $\Delta_3(\lambda)$ samples also the non–random gaps. As $U/t$ increases the gaps close in and for larger and larger $\lambda$ only randomized levels are sampled by $\Delta_3(\lambda)$. The spectral rigidity can thus be used to monitor this regular to random transition in the spectrum. The value $\lambda^*(U/t)$ below which the rigidity has the GOE form grows roughly linear with $U/t$.

**FIG. 1.** The probability distribution $P(s)$ of the level spacings $s$ in the unfolded $5 \times 5$ 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.

To study the statistical properties of the spectrum on larger energy scales we have computed the Wigner-Dyson level rigidity $\Delta_3(\lambda)$ defined as the least square deviation of the level staircase $N_{av}(\epsilon)$ from the best fitting straight line in an interval of length $\lambda$:

$$\Delta_3(\lambda) = \left\{ \frac{1}{\lambda} \min_{(A,B)} \int_{\epsilon_0}^{\epsilon_0+\frac{\lambda}{2}} (N_{av}(\epsilon) - A \epsilon - B)^2 d\epsilon \right\}_{\epsilon_0}. \quad (3)$$

The brackets denote an averaging over $\epsilon_0$. Fig. 3 shows $\Delta_3(\lambda)$ of one specific symmetry sector for five different

**FIG. 2.** The level rigidity $\Delta_3(\lambda)$ of the $(R=6,S=0)$–sector of the $5 \times 5$ Hubbard model for five different values of $U/t$ compared to the random diagonal matrix ensemble (dashed straight line) and to the GOE (full line). For each data set are shown two typical error bars. The error bars grow as a function of increasing $\lambda$ and as a function of decreasing $U/t$.

The level velocity correlation. To obtain a more quantitative measure of the $U/t$–dependence of the spectra, we calculate the level velocity function $c(x)$ [2]. The generalized conductance $C(0) = \langle (\frac{\partial N}{\partial U/t})^2 \rangle_{i,U/t}$ and the rescaled interaction strength $x = \sqrt{C(0)} U/t$ are introduced and $c(x)$ is defined as:

$$c(x) \equiv \left\langle \frac{\partial \xi_i(\bar{x}+x)}{\partial \bar{x}} \frac{\partial \xi_i(\bar{x})}{\partial \bar{x}} \right\rangle_{i,\bar{x}}. \quad (4)$$

It has been found that $c(x)$ is universal for a variety of
single–particle systems with many different external perturbations given that the systems exhibit random matrix behavior \[12] \[14]. Even for some many–body systems the same result has been obtained, and it has been suggested that the spectra of all nonintegrable strongly correlated systems can be classified according to the generalized conductance, mean–level spacing, and Dyson ensemble \[5]. However, we find that this is not the case for the Hubbard model. In Fig. \[3] \( c(x) \) is shown for the representation \((R=6,S=0)\) with \( L = 5 \). This particular representation was chosen since out of its 630 states only 2 were independent of \( U \). It is seen that \( c(x) \) is an exponential decaying function as opposed to the expected generic GOE-curve. In our model the random matrix behavior stems from choosing a sufficiently large value of \( U/t \), e.g. \( U/t = 20 \) as seen by the results of \( P(s) \) and \( \Delta_3(\lambda) \). The parametric change originates from a further change in \( U/t \). We have chosen to do the analysis in the interval \( U/t \in [20,50] \). We can conclude that random matrix behavior of \( P(s) \) and \( \Delta_3(\lambda) \) is not a sufficient criterion for observing universal behavior in the level velocity correlation function for many–body systems. We speculate that GOE–like behavior would be obtained by taking the new symmetry properly into account and, in the case of \( c(x) \), by adding a next–nearest neighbor interaction compatible with the symmetry group to introduce a more rapid and stronger mixing between the levels.

It is important to establish the exact nature of the new symmetry, and to find out if it exists for higher filling factors, where the physical properties of the model are known to be different. In particular it would be interesting to study the regime near half filling and to extend our analysis to more specific Hamiltonians like the \( tJ–\)model and the Heisenberg model. The method presented here is general and can be applied to these models widely used in studies of high temperature superconductivity and magnetism in two dimensions.

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**FIG. 3.** The level velocity correlation function \( c(x) \) (dots) of the \((R=6,S=0)\)–sector of the 5x5 Hubbard model compared to the GOE result (dashed line). The data are obtained with \( U/t \in [20,50] \) for level 350 to 400. Five typical error bars are shown. The insert shows the same data on a semi–logarithmic scale revealing an exponential decay of \( c(x) \) for \( x > 0.2 \).

**Conclusion and discussion.** The existence of a new symmetry in the Hubbard model at low filling has been demonstrated numerically by projecting the Hamiltonian into invariant subspaces of all the known symmetries for a wide range of \( U/t \) and noting how a significant amount of degeneracies persists. The commonly used statistical analysis of random matrix spectra has been applied. A small discrepancy between the actual \( P(s) \) and \( \Delta_3(\lambda) \) the expected random matrix results have been interpreted as a consequence of the new symmetry. We have demonstrated that the Hubbard model is a specific example of a many–body model with strong interaction where, eventhough \( P(s) \) and \( \Delta_3(\lambda) \) are close to the GOE behavior, the parametric dependence \( c(x) \) of the spectra is qualitatively different from random matrix systems. We

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