Localization of interacting fermions at high temperature

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We suggest that if a localized phase at nonzero temperature $T>0$ exists for strongly disordered and weakly interacting electrons, as recently argued, it will also occur when both disorder and interactions are strong and T is very high. We show that in this high-T regime, the localization transition may be studied numerically through exact diagonalization of small systems. We obtain spectra for one-dimensional lattice models of interacting spinless fermions in a random potential. As expected, the spectral statistics of finite-size samples cross over from those of orthogonal random matrices in the diffusive regime at weak random potential to Poisson statistics in the localized regime at strong randomness. However, these data show deviations from simple one-parameter finite-size scaling: the apparent mobility edge "drifts" as the system's size is increased. Based on spectral statistics alone, we have thus been unable to make a strong numerical case for the presence of a many-body localized phase at nonzero T.

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I. INTRODUCTION

Although Anderson's original paper on localization[1] is mostly remembered for its ground-breaking results about single particles in random potentials, one goal of that paper was to learn about transport properties of highly excited many-body eigenstates, e.g., quantum diffusion of nuclear moments. This latter goal was mostly neglected in subsequent research on localization and metal-insulator transitions. However, these questions have been recently brought to our attention by Basko, *et al.*[2] who present detailed arguments that interacting electrons in static random potentials can have a true metal-insulator transition at a nonzero critical temperature. Thus, these systems are argued to have an insulating phase, with strictly zero Ohmic conductivity, even at a nonzero temperature. For some work on these questions published before Basko *et al.* see, for example, Refs. 3–9.

In practice, few transport measurements are possible without first equilibrating the sample with its environment in order to establish a steady state (by removing Joule heat). In metals, this coupling to the environment, provided it is not too strong, does not affect the conductivity (nonlinear transport is another story altogether, see, e.g., Ref. 10). In Anderson insulators, however, the heat bath plays a far less subtle role: it is what permits transport. Conduction occurs by variable-range hopping, which is an inelastic process requiring a heat bath that can locally supply or absorb the energy needed to permit hopping of the charge carriers between localized states that are not precisely degenerate. At the heart of this extreme sensitivity of the dynamics of a localized insulator to the coupling with its environment is its inability to self-equilibrate. It is therefore useful to turn the issue around by distinguishing conductors from true $T>0$ insulators by whether the many-particle system itself constitutes a heat bath. For example, one might ask whether external local probes can deposit limitless amounts of energy or if they tend to saturate the spectrum. Similarly, whether or not attached leads themselves can effectively remove heat from the sample will generally depend on heat conductivity of the sample itself. Thus, we see that whether or not a quantum system of many interacting degrees of freedom constitutes a heat bath is not only a very fundamental question, but also one of some practical relevance.

To the extent that one of the most successful theories of nature, namely, thermodynamics, is founded on the assumption of ergodicity, we expect true insulators (where this assumption is strongly violated) to be rare and require fine tuning of some sort. The noninteracting Anderson insulator is one example, where the unrealistic condition of no interparticle interactions is crucial. Remarkably, the authors of Ref. 2 argue that a nonzero temperature Anderson insulator can be stable against the dephasing effects of interparticle interactions, making this state a sufficiently realistic possibility to be taken seriously and looked for in experiments (provided decoherence from the rest of the universe can be ignored to a good approximation).

The calculations of Ref. 2 are based on a low-energy effective Hamiltonian whose connection with the parameters of the original model of interacting electrons in a random potential could not be established analytically. Thus, it is interesting and likely worthwhile to test their results using other methods and to try to learn more about the nature of the proposed $T>0$ diffusive-to-insulating phase transition and about the range of models that may exhibit it. We report here on one such attempt. To start, we observe that application of the quantitative estimates of the localization transition in Ref. 2 to a lattice model with finite entropy and energy densities (i.e., finite number of states at each site) implies that the aforementioned localized phase and, therefore, the phase transition to the diffusive state can persist all the way to *infinite* temperature. This seemingly innocuous observation has at least two important practical implications. First, by adapting familiar high-temperature expansion techniques, we can more or less rigorously rule out the possibility that such a transition is accompanied by a thermodynamic signature both at infinite temperature and by continuity at any

finite temperature.[11] Perhaps more interestingly, the very large (exponential in volume) number of states available to the system at high temperatures can sometimes create favorable conditions for quickly approaching the thermodynamic limit in various thermodynamic *and* dynamic quantities, which raises the possibility of looking for the signs of this physics numerically, e.g., in exact spectra of finite samples. Our choice of the model and method of analysis are summarized below, followed by results and some preliminary conclusions.

II. ENSEMBLE OF HAMILTONIANS

To reach as large as possible a distance with a given size many-body Hilbert space, we study spinless fermions hopping and interacting on a one-dimensional lattice of L sites with a random potential and periodic boundary conditions. This model has only two states (empty and occupied) per lattice site. The Hamiltonian is

$$H = \sum_i \left[w_i n_i + V\left(n_i - \frac{1}{2}\right)\left(n_{i+1} - \frac{1}{2}\right) \right.$$
$$\left. + c_i^\dagger c_{i+1} + c_{i+1}^\dagger c_i + c_i^\dagger c_{i+2} + c_{i+2}^\dagger c_i \right]. \quad (1)$$

The nearest-neighbor interaction is chosen to be $V=2$, although we have explored other values. The hopping matrix elements to both nearest- and second-neighbor sites are chosen to be $t=t'=1$, although again we have explored other values. The second-neighbor hopping is included so that the model remains nonintegrable (quantum chaotic) and thus diffusive at zero randomness.[12] The on-site potentials w_i are independent Gaussian random numbers with mean zero and variance W^2. Each realization of the disorder potential will generally have mean-square random potential $\sum_{i=1}^L w_i^2/L$ that is not precisely W^2. We have found that restricting our ensemble of samples to those with mean-square random potential *precisely* W^2 reduces our statistical uncertainties by about a factor of 2 in the largest samples. This change of statistical ensembles does produce quantitative changes in the spectral properties (mostly noticeable for intermediate values of disorder, $4 \lesssim W \lesssim 9$), but it does not appear to produce any qualitative changes in the finite-size scaling behavior that would affect our conclusions and it cannot affect the system's intensive properties in the thermodynamic limit.

We study all many-body eigenenergies of this Hamiltonian, weighting them equally; the data shown here are for half-filling $L/2$ particles. Thus, we are studying high temperatures compared to the energy scales of this Hamiltonian. If a localized phase does indeed exist in this model, it should be present even at high T for strong enough disorder. An important motivation for this choice of a model was our recent work[12] on the same model in the absence of randomness, where the approach to thermodynamic limit was rapid enough to observe the onset of hydrodynamic behavior with ≤ 9 particles. Here, we are limited to somewhat smaller sizes, since the random potential violates momentum conservation; we focus on sizes up to $L=16$. The number of realizations needed to achieve adequate statistical certainty depends strongly on W and even more so on L. At $L=8$, we average over 10 000 realizations, whereas at $L=14$, and 16 only about 50–100 suffice *except* in the putative critical region, where we average over 1000 realizations for each W.

III. METHOD OF ANALYSIS

To look for the diffusive-to-insulating phase transition in this model, we have chosen to use what appears to be numerically the most accessible quantity that shows a clear, well-understood difference between the two phases, namely, the spectral statistics of adjacent energy levels of the many-body Hamiltonian. In the localized, insulating phase (assuming it exists in our many-body system), in the thermodynamic limit of a large sample, the eigenstates are localized in the many-body Fock basis of localized single-particle orbitals, so states that are nearby in energy are far apart in this Fock space and do not interact or show level repulsion. As a result, nearby energy levels are simply Poisson distributed.[13] In the diffusive phase, on the other hand, the level statistics of a large sample are those of random matrix theory, the Gaussian orthogonal ensemble (GOE) in particular. For the finite-length samples that we can diagonalize, the level statistics cross over smoothly between these two limiting behaviors as the strength of the random potential is varied. This crossover becomes sharper as the length L is increased, and we can look for a phase transition using standard finite-size scaling techniques; this approach works well for the single-particle localization transition in three dimensions (see, e.g., Ref. 14).

The choice of a quantity to compute and use for the finite-size scaling analysis is to some degree arbitrary: the hypothesis of universality implies that many features of the distribution of eigenvalues of the Hamiltonian are universal in the thermodynamic limit.[13] By analogy to the Binder ratio for phase transitions with a local order parameter,[15] we seek a dimensionless measure of spectral statistical properties, say, $r(W,L)$, that is expected to take different finite values in the thermodynamic limit, $L \to \infty$, in the two phases and at the critical point ($W > W_c$, $W < W_c$, and $W = W_c$). Since the zero of energy is arbitrary, it is natural to work with gaps between many-body levels. Here, in particular, we consider gaps between *adjacent* many-body levels,

$$\delta_n = E_{n+1} - E_n \geq 0,$$

where the eigenvalues of a given realization of the Hamiltonian for a given total number of particles $\{E_n\}$ are listed in ascending order.

The dimensionless quantity we[16] have chosen to characterize the correlations between adjacent gaps in the spectrum is the ratio of two consecutive gaps,

$$0 \leq r_n = \min\{\delta_n, \delta_{n-1}\}/\max\{\delta_n, \delta_{n-1}\} \leq 1.$$

For uncorrelated Poisson spectrum, the probability distribution of this ratio r is $P_P(r) = 2/(1+r)^2$, and its mean value is $\langle r \rangle_P = 2 \ln 2 - 1 \cong 0.386$. The numerically determined probability distribution[17] for large GOE random matrices is shown in Fig. 1; its mean value is $\langle r \rangle_{GOE} = 0.5295 \pm 0.0006$.
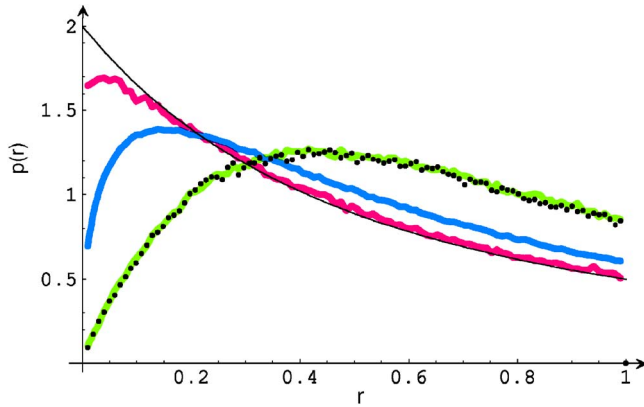
FIG. 1. (Color online) Disorder averaged probability distribution $P(r)$ for Poisson (solid line) and GOE distributed eigenvalues (Ref. 17) (dots) and for our interacting fermion model at randomness $W=3$ in diffusive regime [data in green, mostly overlapping with black (GOE) dots], $W=11$ in localized regime [data in red, mostly overlapping with black (Poisson) line], and $W=7$ in intermediate regime (data in blue) for length $L=16$.

As expected, level repulsion and/or spectral rigidity in the GOE spectra manifests itself in the vanishing of the probability distribution $P_{GOE}(r) \sim r$ as $r \to 0$.

IV. RESULTS

With interaction and hopping terms fixed as above ($t=t'$ $=V/2=1$), we vary the strength of disorder from $W=1$ to $W=10$ or more and for each (L,W) we diagonalize a large number realizations R (see above). For each sample, we compute the spectral average of r $\langle r \rangle$ over *all* states. We then disorder average this quantity $[\langle r \rangle]$ to arrive at $r(W,L)$ exhibited in Fig. 2. The statistical uncertainties in $[\langle r \rangle]$ are estimated as usual as $\pm(([\langle r \rangle^2] - [\langle r \rangle]^2)/(R-1))^{1/2}$.

As expected, larger samples have more Poisson-like statistics than smaller ones for strong disorder, $W > 8$, in an apparently localized regime; while for weak disorder, $W < 4$, the level statistics converge toward GOE with increasing L, since this is the diffusive phase. We have checked that the entire probability distributions $P(r)$ in these regimes approach those of Poisson and GOE spectra (see Fig. 1). In fact, well away from the intermediate range of disorder strength, these universal limiting distributions are reproduced to a high precision by our admittedly limited in size samples. There is an additional crossover at very weak disorder: as crystal momentum conservation is recovered, there appears a turnaround in the statistics as the decoupling of different momentum sectors suppresses the average of r below its GOE value. This latter crossover at weak randomness is a nuisance for us and we steer clear of it the best we can by working away from the clean limit and also not considering very short chains (with less than eight sites) where this momentum pseudoconservation persists to larger values of disorder: $r(W,8)$ shows a remnant of this crossover at $W=1$, while larger values of L do not show it at all over the range of W considered.
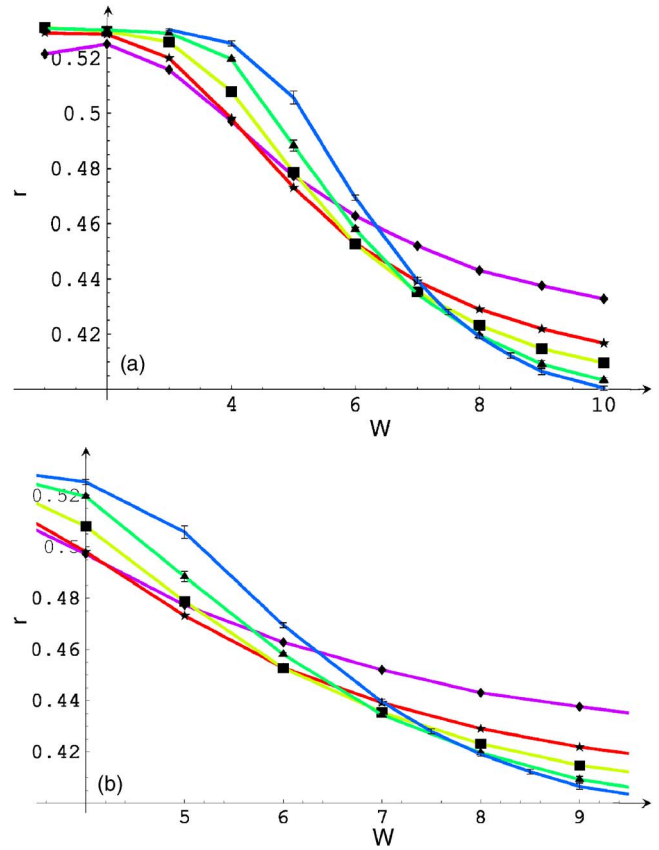

FIG. 2. (Color online) Size L and disorder W dependences of $r(W,L)$. The curves correspond to $L=8$ (diamonds), 10 (stars), 12 (squares), 14 (triangles), 16 (unadorned) from top to bottom for large W. Bottom: an enlargement of the crossing region to make the drift of the crossings more visible. Where not visible, the error bars are smaller than the points.

The simplest one-parameter finite-size scaling scenario for the proposed diffusive-to-insulating phase transition would have these traces of $r(W,L)$ vs W at fixed L in Fig. 2 all cross at W_c as $L \to \infty$, with a slope that increases with increasing L (e.g., see Ref. 14). However, we find that the crossings of the $r(W)$ curves for adjacent L's take place at points that, as L is increased, "drift" progressively toward larger W and smaller (more insulating) r (see Fig. 2). The bottom portion of Fig. 2 displays an enlargement of the intermediate disorder regime, where this drift takes place. Here, we observe that in going from four to five particles, the location of the crossing point shifts by two units of W (horizontal axis), whereas in going from seven to eight particles it is about ≈ 0.5, thus suggesting a trend whereby deceleration of this motion of crossing points persists and results in finite value of W_c as $L \to \infty$ (although further computations will be necessary to support this scenario). It is also interesting to note that vertical displacements of crossing points appear rather substantial, possibly suggesting a limiting value of W_c that is not too different from Poisson (see below).

As this drift precludes the straightforward quantitative analysis of our data in terms of one-parameter scaling theory, we have exerted considerable effort to attempt to eliminate it,[18] including looking at other temperatures, interactions and

fillings, candidate scaling variables other than r, and selective spectral averaging (e.g., excluding states in the high- and low-energy tails of the spectrum). While this drift of the crossings can be reduced (particularly by trimming tails or reducing the temperature), it appears that it is intrinsic to this model's spectral statistics and none of the many things we have tried eliminated or reversed it. Accepting this, there are two very distinct possible implications: either the drift converges to a finite W_c (and likely to $r_c = \langle r \rangle_P$, see below) in the large L limit, or it continues indefinitely to $W_c = \infty$ which would imply that the insulating phase does not exist at these high temperatures. In fact, this latter possibility has already been advocated in previous work, see, e.g., Ref. 5 where it was argued that $W_c(L) \sim L$ [i.e., $W_c(L)$ is a length dependent scale at which spectral statistics changes from Poisson-like to GOE].

Although at this point we cannot choose between these two possibilities based on these data for the spectral statistics, it is worth making some more comments about the former possibility:[18] The apparent drift of the crossing points $\{W_c(L), r_c(L)\}$ is indeed substantial along the *vertical* axis, as would be expected if r_c is converging to the Poisson-limit value $\langle r \rangle_P$. Thus, these data seem consistent with a large L limiting behavior $W_c(L) \rightarrow W_c < \infty$, $r_c(L) \rightarrow \langle r \rangle_P$, whereby the critical point is insulating as far as level statistics are concerned. There are independent reasons, based on analogy to Anderson localization on high dimensional and Cayley graphs,[19] to expect such a behavior. The proposed many-body localization transition is a localization transition in an infinite-dimensional Fock space.[2] Given that there may be plenty of room in that space for the states at a diffusive-to-localized transition (i.e., at the mobility edge) to have an infinite localization length but still have a negligible overlap between states and thus, no level repulsion and Poisson level statistics. This would imply that the spectral statistics should converge to Poisson as L increases both within the localized phase and at the transition, and thus, the "crossings" in our Fig. 2 must move down to $r = \langle r \rangle_P$ in the large L limit. This scenario, with a localized phase for $W > W_c$, seems qualitatively consistent with the data we have presented above. Unfortunately, if this is indeed the case then spectral statistics are not a good tool for simple finite-size scaling analysis. We shall explore other approaches to this problem in the near future.

V. SUMMARY AND OUTLOOK

We have looked for signatures of the proposed many-body localization transition in the statistics of exact spectra of a one-dimensional tight-binding model of strongly interacting spinless fermions in a random potential. Although some indications of this phase transition are clearly seen, there are rather strong deviations from and/or corrections to finite-size scaling present. The latter might be interpreted as calling in to question the existence of the proposed many-body localized phase at the high temperatures we study. Alternatively, this failure of simple one-parameter finite-size scaling might be because the critical point has insulator-like spectral statistics.

In closing, it may be worth noting that thus far we have focused on the most elementary aspects of many-body localization. These may not be necessarily the easiest to study experimentally. Finite-size effects in dynamical response functions, i.e., conductivity, appear more delicate but they are certainly worthwhile understanding, as data may already exist in regimes of interest, in materials as diverse as magnetic salts and disordered conductors.

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[13] The sense in which the eigenvalues are Poisson distributed requires two qualifications. First, the average level spacing varies systematically and substantially within each spectrum; it is exponentially small in volume near the middle and at best power law small in the tails. Second, since the number of random values of the potential is very small compared to the number of

(many-body) levels generated, there are bound to be significant correlations in the latter, even deep inside the insulating phase. However, to the best of our knowledge, these correlations are undetectable provided the thermodynamic limit is taken first before defining and computing statistical measures. Loosely speaking, for a system of L sites, any statistical measure involving a finite number G of consecutive gaps will converge to its Poisson value in the insulating phase as $L \to \infty$.

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[16] The single-gap distribution function, $p(s) = [\langle \delta(s - \delta_n/\langle \delta_n \rangle) \rangle]$, is by far the most commonly used measure of spectral statistics ($\langle \delta \rangle$ is the "local" average gap). Unfortunately, there is substantial ambiguity inherent in choosing an appropriate *definition* of $\langle \delta \rangle$. Different definitions of $\langle \delta \rangle$ we have tried, while each compelling in their own right, all produce additional finite-size effects. To avoid this difficulty, we have opted for a procedure (see main text) that constructs an appropriate statistical measure from the *two-gap* distribution function and does not require defining a local average gap.

[17] GOE data was obtained from 1000 random matrices of size 3432, which is the number of states in a half-filled chain of $L = 14$.

[18] The simplest one-parameter finite-size scaling would have the spectral statistics at the mobility edge intermediate between Poisson and GOE, as appears to be the case for single-particle localization (e. g., Ref. 14). In this case, drifting crossing points would be due to slow decay with increasing L of effects from operators that are irrelevant (in the RG sense) at the critical fixed point. It should be possible then to eliminate or even change the sign of these effects by either changing the observable being studied or the Hamiltonian itself, to cross the phase boundary where the effects due to the irrelevant operators are either quantitatively small or of the opposite sign. However, it is possible that the sign of the irrelevant perturbation is constrained by physical considerations, e.g., in scalar ϕ^4 theory the quartic term is irrelevant above four dimensions but must be positive for the low-temperature phase to exist (the vortex fugacity at the Kosterlitz-Thouless transition in another example, but there it is the high-T phase that needs it). We discuss (in main text) how something along these lines that would invalidate the simplest one-parameter scaling analysis might be responsible for the drift of our crossings in Fig. 2, and for the reason that we have been unable to eliminate or reverse this drift by varying the model or the quantities we measure.

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