Ground state energy of noninteracting fermions with a random energy spectrum

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Abstract –We derive analytically the full distribution of the ground-state energy of K non-interacting fermions in a disordered environment, modelled by a Hamiltonian whose spectrum consists of N i.i.d. random energy levels with distribution $p(\varepsilon)$ (with $\varepsilon \geq 0$), in the same spirit as the "Random Energy Model". We show that for each fixed K, the distribution $P_{K,N}(E_0)$ of the ground-state energy E_0 has a universal scaling form in the limit of large N. We compute this universal scaling function and show that it depends only on K and the exponent α characterizing the small ε behaviour of $p(\varepsilon) \sim \varepsilon^{\alpha}$. We compared the analytical predictions with results from numerical simulations. For this purpose we employed a sophisticated importance-sampling algorithm that allowed us to obtain the distributions over a large range of the support down to probabilities as small as 10^{-160} . We found asymptotically a very good agreement between analytical predictions and numerical results.

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The celebrated "Random Energy Model" (REM) of Derrida [1] has continued to play a central role in understanding different aspects of classical disordered systems, including spin-glasses, directed polymers in random media and many other systems. In the REM, one typically has N energy levels which are considered to be independent and identically distributed (i.i.d.) random variables, each drawn from a probability distribution function (PDF) $p(\varepsilon)$. Typical observables of interest are the partition function, free energy, etc. The REM can also be useful as a toy model in quantum disordered systems. For example, let us consider a single quantum particle in a disordered medium with the Hamiltonian h. We will assume that the spectrum of the operator h has a finite number of states N (for instance a quantum particle on a lattice of finite size and a random onsite potential, as in the Anderson model). In general, solving exactly the spectrum of such an operator is hard, for a generic random potential. One possible approximation, in the spirit of the REM in classical disordered systems, would be to consider the toy model where one replaces the spectrum of the actual Hamiltonian by N ordered i.i.d. energy levels $\varepsilon_1 \leq \varepsilon_2 \leq \cdots \leq \varepsilon_N$ each drawn from the common PDF $p(\varepsilon)$. Without loss of generality, we will also assume that the Hamiltonian \hat{h} has only positive eigenvalues. This would mean that, in the corresponding toy model, the PDF $p(\varepsilon)$ is supported on $[0,+\infty)$. It is well known that, in a strongly disordered quantum system, where all single-particle eigenfunctions are localised in space, the energy levels can be approximated by i.i.d. random variables (see e.g. [2]). Therefore the

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39 REM that we consider here will be relevant in such strongly localised part of the spectrum 40 of a disordered Hamiltonian.

Now consider a system of K noninteracting fermions with the Hamiltonian $\hat{H}_K = \sum_{i=1}^K \hat{h}_i$ where \hat{h}_i is the single particle Hamiltonian associated with the i-th particle. The ground state of this many-body system would correspond to filling up the single particle spectrum up to the Fermi level ε_K , with one particle occupying each of the states with energies $\varepsilon_1, \varepsilon_2, \cdots, \varepsilon_K$. The ground state energy E_0 of this many-body system is therefore given by

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$$E_0 = \sum_{i=1}^K \varepsilon_i \ . \tag{1}$$

Clearly, E_0 is a random variable, which fluctuates from one realisation of the disorder to 47 another. Given $p(\varepsilon)$, we are interested in computing the distribution $P_{K,N}$ of E_0 , for fixed K (i.e. the number of fermions) and N (i.e. the number of levels). We note that, for K=1, $E_0 = \varepsilon_1$ is just the minimum of a set of N i.i.d. random variables and is described by 50 the well-known extreme value statistics [3]. Thus, for general value of K, in particular, it 51 would be interesting to know how sensitive the distribution of E_0 is to the choice of $p(\varepsilon)$. 52 For instance, is there any universal feature of the distribution of E_0 that is independent of 53 $p(\varepsilon)$? We note that E_0 is a sum of random variables, but these random variables are not 54 independent due to the ordering $\varepsilon_1 \leq \varepsilon_2 \leq \cdots \leq \varepsilon_N$ (even though the original unordered 55 random variables are independent). Had they been independent, the sum E_0 in eq. (1), by virtue of the Central Limit Theorem, would converge to a shifted and scaled Gaussian 57 random variable. Here, this is not the case, as the ordering induces non-trivial correlations 58 between these variables. 59

In this paper, we compute exactly the PDF $P_{K,N}(E_0)$ for arbitrary K, N and $p(\varepsilon)$ and show that, indeed, a universal feature emerges in the large N limit. It turns out that the limiting distribution of E_0 , for large N, depends only on the small ε behaviour of $p(\varepsilon) \approx B \varepsilon^{\alpha}$, with $\alpha > -1$, but is otherwise independent of the rest of the features of $p(\varepsilon)$. For fixed α and fixed K, as $N \to \infty$, we show that the distribution of the ground state energy converges to a limiting scaling form

$$P_{K,N}(E_0) \approx b N^{\frac{1}{\alpha+1}} F_K^{(\alpha)} \left(b N^{\frac{1}{\alpha+1}} E_0 \right)$$
 (2)

where $b=(B/(\alpha+1))^{1/(\alpha+1)}$ is just a scale factor. The scaling function $F_K^{(\alpha)}(z)$ (with $z\in[0,+\infty)$) is universal and depends only on α and K. We show that the Laplace transform of $F_K^{(\alpha)}(z)$ is given explicitly by

$$\int_0^\infty F_K^{(\alpha)}(z) e^{-\lambda z} dz = \frac{(\alpha+1)^K}{\Gamma(K)\lambda^{(\alpha+1)(K-1)}} \int_0^\infty x^{\alpha} e^{-\lambda x - x^{\alpha+1}} \left[\gamma(\alpha+1, \lambda x) \right]^{K-1} dx , \quad (3)$$

where $\gamma(a,x) = \int_0^x \mathrm{d}u \, u^{a-1} \mathrm{e}^{-u}$ is the incomplete gamma function. While we can invert formally this Laplace transform (3), it does not have a simple expression for generic α . However, we can derive the asymptotic behaviour of $F_K^{(\alpha)}(z)$

$$F_K^{(\alpha)}(z) \approx \begin{cases} c_1 z^{(\alpha+1)K-1}, & z \to 0, \\ c_2 z^{\alpha} \exp\left[-\left(\frac{z}{K}\right)^{\alpha+1}\right], & z \to \infty, \end{cases}$$

$$(4)$$

where $c_1 = \frac{[\Gamma(\alpha+2)]^K}{\Gamma(K+1)\Gamma((\alpha+1)K)}$ and $c_2 = \frac{(\alpha+1)K^{K-\alpha-2}}{\Gamma(K)}$ are constants. For the extreme-value case K=1 our result, $F_1^{(\alpha)}(z) = (\alpha+1)z^{\alpha}e^{-z^{\alpha+1}}$, coincides with the well known Weibull

scaling function [3]. Note that here we are interested in the sum of K lowest i.i.d. variables supported over $[0, +\infty)$. We remark that in the statistics literature, in a completely different context, the sum of the top K values of a set of i.i.d. random variables with an unbounded support has been studied [4,5]. However, we have not found our results (2) and (3) in the statistics literature.

We start with a set of N positive i.i.d. random variables $\{x_1, x_2, \dots, x_N\}$, each drawn from a common distribution p(x), supported on $[0, +\infty)$. The joint distribution of these variables is simply $P(x_1, \dots, x_N) = \prod_{i=1}^N p(x_i)$. At this stage, these variables are unordered. We are interested in the first K ordered variables $\{\varepsilon_1, \varepsilon_2, \dots, \varepsilon_K\}$ with $K \leq N$. This ordering makes these K variables correlated. Indeed, the joint distribution of the K lowest ordered variables can be written explicitly as

$$P(\varepsilon_1, \cdots, \varepsilon_K) = \frac{\Gamma(N+1)}{\Gamma(N-K+1)} \prod_{i=1}^K p(\varepsilon_i) \prod_{i=2}^K \Theta(\varepsilon_i - \varepsilon_{i-1}) \left[\int_{\varepsilon_K}^{\infty} p(u) \, \mathrm{d}u \right]^{N-K} . \tag{5}$$

This result can be easily understood as follows. We first choose the K distinct variables from an i.i.d. set of N variables. The number of ways this can be done is simply the combinatorial factor $N(N-1)\cdots(N-K+1)=\Gamma(N+1)/\Gamma(N-K+1)$ in eq. (5). The probability that they are ordered is $\prod_{i=1}^K p(\varepsilon_i) \prod_{i=2}^K \Theta(\varepsilon_i-\varepsilon_{i-1})$, where the Heaviside theta functions ensure the ordering. In addition, we have to ensure that the N-K remaining variables are bigger than ε_K , i.e. the largest value among the first K ordered variables. Since these N-K variables are i.i.d., this gives the last factor in eq. (5). The formula in eq. (5) is exact for any $p(\varepsilon)$, K and N. Given the joint PDF (5), we are interested in the distribution $P_{K,N}(E_0)$ of the ground-state energy E_0 in eq. (1). We therefore have

$$P_{K,N}(E_0) = \int P(\varepsilon_1, \cdots, \varepsilon_K) \delta\left(E_0 - \sum_{i=1}^K \varepsilon_i\right) \prod_{i=1}^K d\varepsilon_i .$$
 (6)

The form of this equation naturally suggests to consider the Laplace transform with respect to (w.r.t.) E_0

$$\langle e^{-sE_0} \rangle = \int_0^\infty P_{K,N}(E_0) e^{-sE_0} dE_0.$$
 (7)

Taking the Laplace transform of eq. (6) gives

$$\langle e^{-sE_0} \rangle = \frac{\Gamma(N+1)}{\Gamma(N-K+1)} \int_0^\infty d\varepsilon_K \, p(\varepsilon_K) e^{-s\,\varepsilon_K} \left[\int_{\varepsilon_K}^\infty p(u) du \right]^{N-K} J_{K-1}(\varepsilon_K) \,, \tag{8}$$

where 97

$$J_{K-1}(\varepsilon_K) = \int \prod_{i=1}^{K-1} p(\varepsilon_i) e^{-s\varepsilon_i} d\varepsilon_i \prod_{i=2}^K \Theta(\varepsilon_i - \varepsilon_{i-1}).$$
 (9)

This multiple integral (9) has a nested structure and can be evaluated easily by induction and one gets

$$J_{K-1}(\varepsilon_K) = \frac{1}{(K-1)!} \left[\int_0^{\varepsilon_K} du \, e^{-su} p(u) \right]^{K-1} . \tag{10}$$

Using this result in eq. (8), and also replacing, for later convenience, $\int_y^\infty du \, p(u) = 1 - \int_0^y du \, p(u)$, we get the exact formula

$$\langle e^{-sE_0} \rangle = K \binom{N}{K} \int_0^\infty dy \, p(y) \, e^{-sy} \left[1 - \int_0^y du \, p(u) \right]^{N-K} \left[\int_0^y dv \, p(v) \, e^{-sv} \right]^{K-1} .$$
 (11)

This formula has a simple interpretation. Taking the Laplace transform is equivalent to 102 breaking the system into two species of random variables of size K and N-K (this can be 103 done in $\binom{N}{K}$ ways): Each member of the first species of size K comes with an effective weight $p(\varepsilon) e^{-s\varepsilon}$, while in the second species of size N-K each member comes with an effective 105 weight $p(\varepsilon)$. We first fix the K-th variable to have a value y, whose weight is $p(y) e^{-sy}$. 106 The members of the second species should each be bigger than y (explaining the factor 107 $\left[\int_{y}^{\infty} p(u) du\right]^{N-K}$, while the rest of the (K-1) members of the first species should each be smaller than y, explaining the factor $\left[\int_0^y dv \, e^{-sv} p(v)\right]^{K-1}$. Finally, the biggest variable among the members of the first species can be any of the K members, explaining the factor 109 110 K multiplying the binomial coefficient $\binom{N}{K}$ in eq. (11). With this interpretation, it is clear 111 that eq. (11) can be easily generalized to any linear statistics of the form $L_K = \sum_{i=1}^K f(\varepsilon_i)$ where $f(\varepsilon)$ is an arbitrary function. The ground state energy E_0 considered here corresponds 113 to choosing $f(\varepsilon) = \varepsilon$. For general $f(\varepsilon)$ the effective weight of each member of the first species 114 discussed above is just $p(\varepsilon) e^{-sf(\varepsilon)}$. Hence the formula in eq. (11) generalises to 115

$$\langle e^{-sL_K} \rangle = K \binom{N}{K} \int_0^\infty dy \, p(y) \, e^{-sf(y)} \left[\int_y^\infty p(u) \, du \right]^{N-K} \left[\int_0^y dv \, p(v) \, e^{-sf(v)} \right]^{K-1} . \quad (12)$$

In this paper, we will focus only on the case $f(\varepsilon) = \varepsilon$. Below, we thus start with the exact result in eq. (11) and analyse its behaviour in the large N limit.

To understand the large N scaling limit, it is instructive to start with the K=1 case. In this case, $E_0 = \varepsilon_1$ is just the minimum of a set of N i.i.d. random variables, each drawn from $p(\varepsilon)$. In this case, eq. (11) reads (upon setting K=1)

$$\langle e^{-sE_0} \rangle = N \int_0^\infty dy \, p(y) \, e^{-sy} \left[1 - \int_0^y du \, p(u) \right]^{N-1} ,$$
 (13)

where we replaced $\int_y^\infty \mathrm{d}u\, p(u) = 1 - \int_0^y \mathrm{d}u\, p(u)$, using the normalisation of p(u). In the large N limit, the dominant contribution to the integral over y comes from the regime of y where the integral $\int_0^y \mathrm{d}u\, p(u)$ is of order O(1/N). For other values of y, the contribution is exponentially small in N, for large N. Hence, we see that, in the large N limit, only the small y behaviour of p(y) matters. Let

$$p(y) \underset{y \to 0}{\approx} B y^{\alpha} \tag{14}$$

where $\alpha > -1$ in order that p(y) is normalisable and clearly B > 0. Substituting this leading order behaviour of p(y) for small y (14) in eq. (13), we get

$$\langle e^{-sE_0} \rangle \approx B N \int_0^\infty dy \, y^\alpha \, e^{-sy} \exp\left(-\frac{B N}{\alpha + 1} \, y^{\alpha + 1}\right).$$
 (15)

Performing the change of variable $y = \left(\frac{\alpha+1}{BN}\right)^{\frac{1}{\alpha+1}} x$, we get

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$$\langle e^{-sE_0} \rangle \approx (\alpha + 1) \int_0^\infty dx \, x^\alpha \exp\left(-\frac{s}{h N^{\frac{1}{\alpha+1}}} x - x^{\alpha+1}\right),$$
 (16)

where $b=(B/(\alpha+1))^{1/(\alpha+1)}$. Inverting the Laplace transform formally, we obtain the scaling form given in eq. (2) with K=1 and the scaling function $F_1^{(\alpha)}(z)$ has its Laplace transform as in (3) with K=1. Inverting this Laplace transform exactly, we recover the Weibull scaling function $F_1^{(\alpha)}(z)=(\alpha+1)z^{\alpha}\,\mathrm{e}^{-z^{\alpha+1}}$. The calculation for K=1 shows that only the small y behaviour of p(y) matters in the limit of large N. Furthermore, for K=1, we see that the typical value of E_0 scales as $N^{-\frac{1}{\alpha+1}}$ for large N. We then anticipate that,

even for K > 1, the typical scale of E_0 will remain the same $E_0 \sim N^{-\frac{1}{\alpha+1}}$ for large N. Below, we indeed use this typical scale for E_0 (and verify a posteriori) and compute the scaling function $F_K^{(\alpha)}(z)$ for general K in eq. (2).

We now derive the main results in Eqs. (2) and (3) for all $K \geq 1$. Anticipating the scaling $E_0 \sim N^{-\frac{1}{\alpha+1}}$ as mentioned above, we set

$$E_0 = \frac{1}{b} N^{-\frac{1}{\alpha+1}} z , \qquad (17)$$

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where b is a constant to be fixed later and the scaled ground state energy z is of order O(1). Substituting this scaling form (17) in eq. (11), we see that the left hand side (l.h.s.) reads, $\langle e^{-sE_0} \rangle = \langle e^{-s\,N^{-\frac{1}{\alpha+1}}\,z/b} \rangle = \langle e^{-\lambda\,z} \rangle$ where $\lambda = N^{-\frac{1}{\alpha+1}}\,s/b$ is the rescaled Laplace variable. We will take the $N \to \infty$ limit, keeping λ fixed. This then corresponds to $s \to \infty$ limit. On the right hand side (r.h.s.) of eq. (11) we make a change of variable $s\,y = \tilde{x}$ as well as $u = \tilde{u}/s$ and $v = \tilde{v}/s$. This gives

$$\langle e^{-\lambda z} \rangle = \frac{K}{s^K} \binom{N}{K} \int_0^\infty d\tilde{x} \, p\left(\frac{\tilde{x}}{s}\right) e^{-\tilde{x}} \left(1 - \frac{1}{s} \int_0^{\tilde{x}} d\tilde{u} \, p\left(\frac{\tilde{u}}{s}\right)\right)^{N-K} \left(\int_0^{\tilde{x}} d\tilde{v} \, p\left(\frac{\tilde{v}}{s}\right) e^{-\tilde{v}}\right)^{K-1}. \tag{18}$$

In the large s limit, we use $p(y) \approx B y^{\alpha}$ to leading order. Inserting this behaviour in eq. (18), we get

$$\langle e^{-\lambda z} \rangle \approx \frac{K B^K}{s^{(\alpha+1)K}} {N \choose K} \int_0^\infty d\tilde{x} \, \tilde{x}^\alpha \, e^{-\tilde{x}} \left(e^{-\frac{B(N-K)}{(\alpha+1) \, s^{\alpha+1}} \, \tilde{x}^{\alpha+1}} \right) \left[\gamma(\alpha, \tilde{x}) \right]^{K-1} \tag{19}$$

where we recall that $\gamma(a,x) = \int_0^x du \, u^{a-1} e^{-u}$ is the incomplete gamma function. We now use $s = (\lambda b) N^{\frac{1}{\alpha+1}}$ and choose

$$b = \left(\frac{B}{\alpha + 1}\right)^{\frac{1}{\alpha + 1}} . \tag{20}$$

Furthermore, in the large N limit $K\binom{N}{K} \sim N^K/\Gamma(K)$. Using these results, and rescaling $\tilde{x} = \lambda x$, we arrive at

$$\langle e^{-\lambda z} \rangle = \frac{(\alpha + 1)^K}{\Gamma(K)\lambda^{(\alpha+1)(K-1)}} \int_0^\infty x^\alpha e^{-\lambda x - x^{\alpha+1}} \left[\gamma(\alpha + 1, \lambda x) \right]^{K-1} dx.$$
 (21)

This clearly shows that the distribution of the rescaled random variable $z=(E_0\,b)\,N^{\frac{1}{\alpha+1}}$ [see eq. (17)] converges to an N-independent form $F_k^{(\alpha)}(z)$ for large N, whose Laplace transform is given by $\int_0^\infty F_K^{(\alpha)}(z) \mathrm{e}^{-\lambda z} \,\mathrm{d}z = \langle \mathrm{e}^{-\lambda z} \rangle$. Therefore eq. (21) demonstrates the result announced in eq. (3).

Special cases $\alpha = 0$. In this case eq. (3), using $\gamma(1, \lambda x) = 1 - e^{-\lambda x}$, reduces to

$$\int_0^\infty F_K^{(0)}(z) e^{-\lambda z} dz = \frac{1}{\Gamma(K)\lambda^{K-1}} \int_0^\infty dx \, e^{-(\lambda+1)x} \left(1 - e^{-\lambda x}\right)^{K-1} = \frac{\Gamma(1+1/\lambda)}{\lambda^k \Gamma(k+1+1/\lambda)} . (22)$$

Using the properties of the Γ function, one can express the r.h.s. of (22) as a simple product

$$\int_0^\infty F_K^{(0)}(z) e^{-\lambda z} dz = \prod_{m=1}^K \frac{1}{1 + m \lambda}.$$
 (23)

To invert this Laplace transform, we note that the r.h.s. has simple poles at $\lambda = -1/m$ with $m = 0, 1, \dots, K$. Evaluating carefully the residues at these poles, we can invert this Laplace transform explicitly and get

$$F_K^{(0)}(z) = \sum_{n=1}^K (-1)^{K-n} \frac{n^{K-1}}{(K-n)! \, n!} e^{-z/n} . \tag{24}$$

For instance,

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$$F_1^{(0)}(z) = e^{-z} \tag{25}$$

$$F_2^{(0)}(z) = e^{-z/2} - e^{-z}$$
 (26)

$$F_3^{(0)}(z) = \frac{3}{2}e^{-z/3} - 2e^{-z/2} + \frac{1}{2}e^{-z}.$$
 (27)

Numerical simulations. Next, we verify our analytical predictions via numerical simulations. 156 To test the prediction of the scaling behaviour in eq. (2), as well as to test the universality of 157 the associated scaling function $F_K^{(\alpha)}(z)$, we consider four different distributions for the energy levels: (a) an exponential distribution $p(\varepsilon) = e^{-\varepsilon} \Theta(\varepsilon)$, (b) an half-Gaussian distribution 158 159 $p(\varepsilon) = \sqrt{\frac{2}{\pi}} e^{-\varepsilon^2} \Theta(\varepsilon)$, (c) a Pareto distribution $p(\varepsilon) = \frac{2}{\varepsilon^3} \Theta(\varepsilon - 1)$ and (d) $p(\varepsilon) = \varepsilon e^{-\varepsilon} \Theta(\varepsilon)$. 160 The cases (a) and (b) clearly correspond to $\alpha = 0$. Hence we expect the scaling function to be given by $F_K^{(0)}(z)$ in eq. (24). The Pareto case (c), with support over $[1, +\infty)$, also corresponds to the $\alpha = 0$ case, as seen easily after a trivial shift $\varepsilon \to \varepsilon - 1$. Hence, in 163 this case as well, we expect the scaling function to be given by $F_K^{(0)}(z)$. However, case (d) is different as it corresponds to zis different as it corresponds to $\alpha = 1$ and hence the scaling function should be given by 165 $F_K^{(1)}(z)$. In fig. 1, we compare the simulation results with the analytical predictions and find very good agreement. Note that in cases (a)-(c), the scaling function $F_K^{(0)}(z)$ has an explicit expression as in eq. (24). Hence, it is easy to compare directly the simulation results with 168 this expression (as in fig. 1 (a)-(c)). However, for case (d), where $\alpha = 1$, we do not have a 169 simple explicit formula for $F_K^{(1)}(z)$, though we have explicitly given its Laplace transform in 170 eq. (3) with $\alpha = 1$. Hence, to compare with the simulation results, we first needed to invert 171 this Laplace transform using an arbitrary precision library [21]. This comparison is shown 173

To obtain the presented numerical results one has to generate N random numbers according to the desired probability density $p(\varepsilon)$. This is done by a standard method, namely we first choose a uniform random number $\eta \in [0,1]$ and then generate ε using the formula, $\int_0^\varepsilon p(\varepsilon') \, \mathrm{d}\varepsilon' = \eta$. The exponential (a) and Pareto (c) case can be trivially obtained using this relation [6]. In the half-Gaussian case (b), the Gaussian random numbers can be generated using the Box-Muller method [6]. In the case (d), $p(\varepsilon) = \varepsilon \mathrm{e}^{-\varepsilon}$, the above relation reads $\eta = \int_0^\varepsilon p(\varepsilon') \mathrm{d}\varepsilon' = 1 - (1+\varepsilon)\mathrm{e}^{-\varepsilon}$, which can also be inverted using the -1 branch of the Lambert W function [8] $\varepsilon = -W_{-1}\left(\frac{\eta-1}{\varepsilon}\right) - 1$. To evaluate the Lambert W function, we use the GSL implementation [7].

The sum E_0 in eq. (1) is completely determined by the values $\eta = (\eta_1, \dots, \eta_N)$. If one simply generates many times vectors η of independent uniform random numbers and correspondingly obtained random numbers $(\varepsilon_1, \dots, \varepsilon_N)$, one will obtain only typical results for E_0 , *i.e.* those having a high enough probability. Here, we sample the distributions over a broad range of the support, also in the far tails, where the probabilities are extremely small. For this purpose, we use a well tested importance sampling scheme [9, 10]. Here the vectors η are sampled using the Metropolis algorithm including a bias of samples away from the main part of the distribution. We use a bias $e^{-E_0/T}$, where T is a "temperature" parameter which can be positive and negative and allows us to address different ranges of the distribution. Since the bias is known, the Metropolis results can be corrected for the

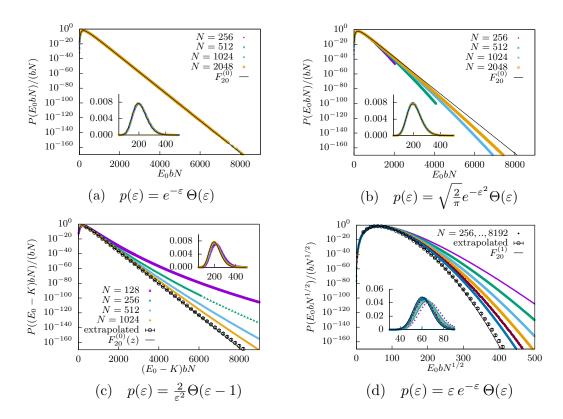


Fig. 1: (colour online) Scaled distribution $P_{K,N}(E_0)$ for K=20, for different values of N and for four different distribution $p(\varepsilon)$. The insets show the behaviour near the peaks for the four different cases. (a) shows exponentially distributed $p(\varepsilon)=\mathrm{e}^{-\varepsilon}\,\Theta(\varepsilon)$ which corresponds to $\alpha=0$ and b=1 [see eq. (2)]. The scaling function $F_{K=20}^{(0)}$ in eq. (24) matches very well the numerical data all the way up to the tails. (b) shows half-Gaussian distributed $p(\varepsilon)=\frac{\sqrt{2}}{\sqrt{\pi}}\mathrm{e}^{-\varepsilon^2/2}\,\Theta(\varepsilon)$ corresponding to $\alpha=0$ and $b=p(0)=\frac{2}{\sqrt{2\pi}}$. (c) shows Pareto distributed energy levels $p(\varepsilon)=\frac{2}{\varepsilon^3}\Theta(\varepsilon-1)$. After shifting $\varepsilon\to\varepsilon-1$, i.e. $E_0\to E_0-K$, this falls in the $\alpha=0$ universality, with b=2. In this case, using the finite-size extrapolation scheme shown in black circles (see text and eq. (30) with $\beta=1$), the data approach the theoretical scaling function $F_{20}^{(0)}(z)$. (d) shows energy levels distributed according to $p(\varepsilon)=\varepsilon\mathrm{e}^{-\varepsilon}\,\Theta(\varepsilon)$. This corresponds to the $\alpha=1$ universality class, with the scaling parameter $b=1/\sqrt{2}$. Again, using the finite-size scaling form (see text and eq. (30)) with $\beta=1/2$, the extrapolated data (shown in black circles) match well with the theoretical scaling function $F_{20}^{(1)}(z)$, obtained from the numerical Laplace inversion of eq. (3), setting K=20 and $\alpha=1$.

bias to obtain the actual distribution. This enables us to gather good statistics also in the far tails.

To be more concrete, we use a Markov chain $\eta(t) = \eta(0), \eta(1), \ldots$ Every move $\eta(t) \to \eta(t+1)$ consists of changing one entry of $\eta(t)$ leading to a trial η' ("local update"). While the most simple method to change would be the replacement of one uniform-distributed random number by a freshly drawn one, as used in Ref. [10], this will lead to difficulties especially for small values K. For the far tails, there will be a point where all entries of η are almost one (or almost zero) and almost every new proposal will be rejected, since it is improbable to draw a random number very close to the previous one. Therefore we perform a slightly more involved protocol, where instead of redrawing we change an entry $\eta_i \to \eta_i + \xi \delta$, where $\xi \in [-1, 1]$ is uniformly distributed and $\delta \in \{10^{-i} | i \in \{0, 1, 2, 3, 4, 5\}\}$ with uniform probability 1/6. Thus δ determines the scale of the local change. Changes resulting in an entry $\eta_i \notin [0, 1)$ are directly rejected, i.e. $\eta(t+1) = \eta(t)$. Note that this

protocol will still result in uniformly distributed random numbers η_i , if every change in [0,1) was accepted, i.e. $\eta(t+1) = \eta'$. Here each proposed change is accepted instead with the Metropolis acceptance ratio

$$p_{\rm acc} = \min\{1, e^{-\Delta E_0/T}\},$$
 (28)

where ΔE_0 is the change in energy caused by the proposed change, and otherwise also rejected.

For any value of T, as usual for Monte Carlo simulations, performing these Markov chains "long enough" and taking measurements, this results in a histogram $P_T(E_0)$ for each temperature, which can be corrected for the bias using

$$P(E_0) = e^{E_0/T} Z(T) P_T(E_0). (29)$$

The a-priori unknown normalization parameter Z(T) can be obtained by enforcing continuity and normalization of the whole distribution, which is obtained from performing simulations for several values of T, including $T=\infty$, which corresponds to simple sampling. We will not go into further details, since this algorithm is well described in several other publications [9–11].

For the Pareto distributed case $p(\varepsilon) = \frac{2}{\varepsilon^3}\Theta(\varepsilon-1)$, we used instead of the aforementioned sampling with bias $e^{E_0/T}$ a modified Wang-Landau sampling [12–16] with multiple histograms and subsequent entropic sampling [17,18]. We used Wang Landau sampling for this case, since the temperatures are harder to adjust, *i.e.* for negative temperatures it happens quickly that equilibration becomes impossible and the energy increases constantly. This effect is already known to pose difficulties for the aforementioned sampling with bias [19,20].

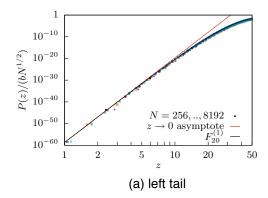
We set K=20 in fig. 1 and compare the distribution $P_{K=20,N}(E_0)$ for different values of N. We verify, by a data collapse, the scaling form predicted in eq. (2) and also compare the numerical scaling function to the analytical ones. As mentioned earlier, for the $\alpha=0$ case (corresponding to cases (a)-(c)), the analytical scaling function is given in eq. (24). For the $\alpha=1$ (corresponding to case (d)), we invert the Laplace transform in eq. (3) for K=20 and $\alpha=1$, using an arbitrary precision library [21].

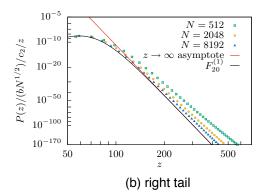
While the exponential case fits very well to the analytic result even for small values of N, the other cases show strong finite-size effects especially in the extreme right tail. Such finite-size effects are known to occur frequently in the extreme statistics of i.i.d. random variables [22]. As seen in fig. 1, the discrepancy between the numerical and the analytical results is very small in the main region (i.e. in the bulk). In the tails, we need to use a finite-size ansatz to study the convergence of the numerical results as $N \to \infty$. For example, it is natural to expect that the finite-size corrections to the leading scaling form in eq. (2) is of the form

$$P_{K,N}(E_0) = b N^{1/(1+\alpha)} \left[F_K^{(\alpha)}(z) + N^{-\beta} G_K^{(\alpha)}(z) + N^{-2\beta} H_K^{(\alpha)}(z) + \dots \right] , \tag{30}$$

where $\beta = \min(1/(1+\alpha), 1)$, $z = b N^{1/(\alpha+1)} E_0$ is the scaling variable, and $G_K^{(\alpha)}(z)$, $H_K^{(\alpha)}(z)$ describe the finite-size scaling of the correction terms. Thus for $\alpha = 0$ one has $\beta = 1$, while for $\alpha = 1$, we have $\beta = 1/2$. For several values of z, we extrapolate the data by fitting pointwise the numerical data in fig. 1 as a function of N, to obtain estimates for the asymptotes $F_K^{(\alpha)}(z)$. We treated the cases (c) (corresponding to $\alpha = 0$, and hence $\beta = 1$) and (d) ($\alpha = 1$, $\beta = 1/2$), the extrapolated values are shown as symbols. Furthermore, in fig. 2, we show the behaviour in the tails for the case (d), which exhibits the strongest finize-size effects, such that the asymptotic behaviour eq. (4) is directly visible. It is apparent that the convergence for large values of N is faster in the left tail $z \to 0$, while it is much slower in the right tail $z \to \infty$.

Conclusion. In this paper, we have studied analytically and numerically the full distribution of the ground-state energy of K non-interacting fermions in a disordered environment,





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Fig. 2: (colour online) We consider the tails of the distribution $P_{K=20,N}(E_0)$ for the case $p(\varepsilon) = \varepsilon e^{-\varepsilon}$, corresponding to $\alpha = 1$. This scaling function in this case is given by $F_{K=20}^{(1)}(z)$. The asymptotic behaviors of $F_{K=20}^{(1)}(z)$ in eq. (4), for $z \to 0$ (left tail, in (a)) and $z \to \infty$ (right tail in (b)) are compared to numerical simulations. The data have been plotted on a scale such that the two cases from eq. (4) appear as straight lines. In (b), for clarity, only three different values of N have been plotted.

modelled by a Hamiltonian whose spectrum consists of N i.i.d. random energy levels with distribution $p(\varepsilon)$ (with $\varepsilon \geq 0$), in the same spirit as the "Random Energy Model". This ground state energy is the sum of the smallest K values drawn from a probability distribution and therefore a generalization of the extrem-value statistics, which corresponds to the case K=1. Thus our results should be of interest also in a very general mathematical context.

We have shown that for each fixed K, the distribution $P_{K,N}(E_0)$ of the ground-state energy has a universal scaling form in the limit of large N (see eq. (2)). This universal distribution depends only on K and the exponent α characterizing the small ε behaviour of $p(\varepsilon) \sim \varepsilon^{\alpha}$. We derive an exact expression for the Laplace transform of this scaling function in eq. (3). For generic α , the asymptotic behaviors of the scaling function are derived explicitly in eq. (4), while for the special case $\alpha = 0$, the Laplace transform can be explicitly inverted, giving the full scaling function in eq. (24). Numerically, while the peak region of the distribution of E_0 can be easily estimated by standard methods, estimating the tails of the distribution where the probability is very small is hard and requires more sophisticated techniques. In this paper, using an importance sampling algorithm, we were able to estimate the tail probabilities (up to a precision as small as 10^{-160}) and thereby to verify the theoretical predictions. Thus the main conclusion of our work is that, even though the individual energy levels are independent random variables, the ordering needed to compute the ground-state energy induces effective correlations between the energy levels. These effective correlations then lead, for the ground-state energy, to a whole new class of universal scaling functions parameterised by K and α .

In this work, we have modelled the single-particle energy levels of a quantum disordered system by i.i.d. random variables, à la REM. This REM approximation for the energy levels is known to be valid for disordered Hamiltonians whose eigenstates are strongly localised in space [2]. Thus we expect that the results presented in this paper for the universal distribution of the ground state energy would apply to such strongly disordered quantum systems. It is then natural to ask what happens to the ground-state energy for Hamiltonians with weakly localised eigenstates. In some weakly localised systems, a description based on Random Matrix Theory (RMT) [2] is a good approximation, where the energy levels (identified with the eigenvalues of a random matrix) are strongly correlated with mutual level repulsion. In this RMT context, several linear statistics of ordered eigenvalues have been

recently introduced and studied for large N under the name of truncated linear statistics (TLS) [23, 24]. The ground-state energy in eq. (1) or more generally the linear statistics as in eq. (12) studied here are instances of TLS, but for i.i.d. random variables. It would thus be interesting to see how the TLS, studied here for i.i.d. variables, crosses over to the RMT case, as one goes from the strongly localised part of the spectrum of a disordered Hamiltonian to the weakly localised part.

* * *

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