Renormalization approach for the two-dimensional Anderson model at the band edge: Scaling of the localization volume

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We study the localization volumes V (participation ratio) of electronic wave functions in the 2*d*-Anderson model with diagonal disorder. Using a renormalization procedure, we show that at the band edges, i.e., for energies $E \approx \pm 4$, V is inversely proportional to the variance $\langle \epsilon^2 \rangle$ of the site potentials. Using scaling arguments, we show that in the neighborhood of $E = \pm 4$, V scales as $V = \langle \epsilon^2 \rangle^{-1}g((4-|E|)/\langle \epsilon^2 \rangle)$ with the scaling function g(x). Numerical simulations confirm this scaling ansatz.

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I. INTRODUCTION

A large amount of work has been done in the past decades to understand the localization behavior in randomly disordered systems. The standard model for a single-particle electronic wave function in tight binding approximation in the presence of disorder is the Anderson model.^{1–3} In d=2 and with diagonal disorder, it can be written as

$$\psi_{n+1,m} + \psi_{n-1,m} + \psi_{n,m+1} + \psi_{n,m-1} - 4\psi_{n,m}$$

= $(E-4)\psi_{n,m} - \epsilon_{n,m}\psi_{n,m}.$ (1)

Here *E* is the energy, the hopping potentials between nearest neighbor are all set to unity, (n,m) are the site indices, ψ is the eigenfunction, and $|\psi_{n,m}|^2$ is the probability to find an electron at site (n,m). The $\epsilon_{n,m}$ are the site potentials which are all uncorrelated random numbers with the variance $\langle \epsilon^2 \rangle \equiv (1/N^2) \sum_{n,m=1}^N \epsilon_{n,m}^2$. Their average value $\langle \epsilon \rangle \equiv (1/N^2) \sum_{n,m=1}^N \epsilon_{n,m}$ is set equal to zero. The term $-4\psi_{n,m}$ on both sides of Eq. (1) is explicitly written down in order to show the discretized Laplace operator on the left-hand side of the equation, that describes the hopping terms (see below).

It has been long recognized that in d=1 and d=2 all eigenstates of Eq. (1) are localized, whereas a localization-delocalization transition occurs in d=3. However, the shape of the wave functions and the value of the localization length $\lambda(E, \langle \epsilon^2 \rangle)$ is still being discussed.

In d=1 and for uncorrelated site potentials, exponential localization was proven throughout the energy band^{1,4,5} and a lot of rigorous results and scaling theories exist for the localization length λ , defined via the Lyapunov exponent. Close to the band edges (i.e., at $E=\pm 2$ in d=1), a weak disorder expansion yields

$$\lambda = \langle \epsilon^2 \rangle^{-\alpha} f \left(\frac{E_c - |E|}{\langle \epsilon^2 \rangle^{\beta}} \right) \tag{2}$$

with $E_c=2$, $\alpha=1/3$, and $\beta=2/3$.^{6,7} Recently, it has been shown by a space renormalization procedure^{8,9} that Eq. (2) also holds for the case of long-range correlated site potentials with correlation exponent γ , $0 < \gamma \le 1$. In this case, the exponents must be replaced by $\alpha=1/(4-\gamma)$ and $\beta=2/(4-\gamma)$ and $\gamma=1$ refers to the uncorrelated case of Refs. 6 and 7. At the band center on the other hand, a different behavior of λ occurs. A Green's function technique¹⁰ yields $\lambda \sim \langle \epsilon^2 \rangle^{-1}$ for E=0 and in some distance from the band center, a secondorder perturbation theory of the diagonal elements of the Green's function^{1,11} yields $\lambda(E) \sim (4-E^2)/\langle \epsilon^2 \rangle$.

For d=2, on the other hand, no analytical theory for the localization behavior is known yet. Numerical simulations close to the band center exist on the basis of Green's functions calculations,¹² exact diagonalization,¹³ and the Lanczos algorithm,¹⁴ but do not lead to an exact or scaling form of λ or related quantities. Moreover, it was shown in Ref. 14, that the wave function in the two-dimensional Anderson model does not decay exponentially. Instead, a subexponential decay of ψ was found with λ increasing logarithmically with the distance *r* from the localization center.

In this paper, we concentrate on the band edges, i.e., on energies $E \approx \pm 4$ of the Anderson model in d=2 with uncorrelated potentials. We develop a renormalization approach, similar to the one in d=1 of Refs. 8 and 9 and use it to find a scaling form for the localization volume V, which is related to the inverse participation ratio P^{-1} . In d=2 and with the wave function $\psi_{n,m}$ being normalized by $\sum_{n,m} \psi_{n,m}^2 = 1$, P^{-1} is defined by^{15,16}

$$P^{-1} = \sum_{n,m=1}^{N} |\psi_{n,m}|^4.$$
(3)

Its inverse value *P* is a *d*-dimensional volume and measures the extension of a given state. If we divide *P* by the volume V_0 of the system, we get the relative volume *V* of the eigenstate, $V \equiv P/V_0$, i.e., the portion of the system where the wave amplitude is large. It can be easily verified that in d=1,2 or 3, $V \sim \lambda^d$ for all wave functions of the form $\psi(r) \sim \exp[-(r/\lambda)^{\Phi}]$, $\Phi > 0$. Therefore, one can define an effective localization length $V^{1/d} \sim \lambda$, which measures the average diameter of the state. For numerical calculations in d=2 and d=3, where the wave functions do not decay exponentially, *V* is easier accessible than λ and therefore, we focus on *V* in this paper.

Since $V \sim \lambda$ in d=1, Eq. (2) holds up to an irrelevant proportionality factor also for V. It is the purpose of this paper to show that a similar scaling law as the one of Eq. (2) holds also for V in d=2,

$$V = \langle \epsilon^2 \rangle^{-\alpha} g \left(\frac{E_c - |E|}{\langle \epsilon^2 \rangle^\beta} \right) \tag{4}$$

but with different exponents, $\alpha = 1$ and $\beta = 1$, and with $E_c = 4$. This scaling ansatz is confirmed by numerical calculations.

The paper is organized as follows: In Sec. II we explain the outline of the renormalization approach, while in Sec. III the scaling ansatz for the localization volume V is developed and tested by numerical simulations. Additional remarks about former renormalization theories and the extension to the vibrational problem are given in Sec. IV.

II. THE RENORMALIZATION APPROACH

In the renormalization approach, we want to combine single sites of the lattice to blocks. This procedure must be reasonable in the limit of small values of 4-|E|, i.e., close to the band edges. In this context, we must recall that the wave functions possess two characteristic length scales, (i) the wavelength Λ of the ordered lattice that describes the periodic fluctuating part of the wave function and (ii) the localization length that describes their decaying envelope. As in d=1,⁹ we assume that the periodic part of ψ does not depend on the disorder but is reminiscent of the functions of an ordered lattice, where the disorder terms $\epsilon_{i,j}$ are zero and ψ is a regular sin or cos function. By solving Eq. (1) for the ordered case, we found in d=1 that $\Lambda^2 \sim (|E_c|-E)^{-1}$. In d=2, with the wavelengths Λ_x and Λ_y in x and y direction, respectively, we have

$$\Lambda_x^2 \ge (E_c - |E|)^{-1} \text{ and } \Lambda_y^2 \ge (E_c - |E|)^{-1},$$
 (5)

where $E_c=4$. At the band edges, Λ diverges and the wave function no longer resolves the details of the disorder potentials. In this case, we can imagine that neighboring sites of the lattice move as blocks and the following renormalization approach becomes legitimate.

In the following, we consider the upper band edge E=4, but by canceling the terms $-4\psi_{n,m}$ on both sides of Eq. (1) and taking into account that the $\epsilon_{n,m}$ are randomly distributed around their mean value of $\langle \epsilon \rangle = 0$, we can see that the equation is symmetric under the transformation $E \rightarrow -E$. Therefore, the renormalization approach is also valid for the lower band edge E=-4.

In order to transform Eq. (1) into block form, we first replace the site indices (n,m) of the central site in Eq. (1) (see also Fig. 1) successively by (n+1,m), (n-1,m), (n,m+1), and (n,m-1). Combining those four equations with Eq. (1) and rearranging the terms, we arrive at

$$\begin{split} \psi_{n+2,m} + \psi_{n-2,m} + \psi_{n,m+2} + \psi_{n,m-2} - 4\psi_{n,m} \\ &= -(4f_{n,m} + f_{n,m+1} + f_{n,m-1} + f_{n+1,m} + f_{n-1,m}) \\ &+ (E-4)(4\psi_{n,m} + \psi_{n+1,m} + \psi_{n-1,m}) \\ &+ \psi_{n,m+1} + \psi_{n,m-1}) + 8\psi_{n,m} \\ &- 2(\psi_{n+1,m+1} + \psi_{n+1,m-1} + \psi_{n-1,m+1} + \psi_{n-1,m-1}), \quad (6) \end{split}$$

with the abbreviation $f_{i,j} \equiv \epsilon_{i,j} \psi_{i,j}$. Comparing this result with



FIG. 1. Sketch of the Anderson lattice according to Eqs. (1) and (8) as explained in the text. The circles represent the different lattice sites, the straight lines between them indicate the usual nearest-neighbor coupling, whereas the couplings of Eq. (8) are shown by the oval lines. The black circles stand for the site potentials that form the block potential [see Eq. (9)].

Eq. (1), we can see that the left-hand side of Eq. (6) is again a Laplace operator, but with twice the distance between $\psi_{n,m}$ and its neighbors. The first two terms on the right-hand side, involving the disorder terms $f_{i,j}$ and the eigenvalue (4-E), are similar to the corresponding terms in Eq. (1), with the only difference that they no longer depend on a single site (n,m) but couple sites at distances <2 from (n,m) to blocks.

The last two terms, however, involve couplings between $\psi_{n,m}$ and its second nearest neighbors $\psi_{n+1,m+1}$, $\psi_{n+1,m-1}$ and so on and do not occur in Eq. (1) (nor in the corresponding derivation in d=1). Using a Taylor expansion that holds in third order, we approximate these terms by

$$\begin{split} \psi_{n+1,m+1} + \psi_{n+1,m-1} + \psi_{n-1,m+1} + \psi_{n-1,m-1} \\ &\approx -4\psi_{n,m} + 2(\psi_{n+1,m} + \psi_{n-1,m} + \psi_{n,m+1} + \psi_{n,m-1}) \\ &= 4\psi_{n,m} - 2f_{n,m} + 2(E-4)\psi_{n,m}, \end{split}$$
(7)

where Eq. (1) has been inserted in the last step. This approximation is consistent with the standard interpretation of the left-hand side of Eq. (1) as a discretized Laplacian operator, which approximates $\Delta \psi$ by the same kind of Taylor expansion and with the same error bars of the order $O(a^4)$, where *a* is the lattice constant. Inserting Eq. (7) into Eq. (6) we finally arrive at

$$\begin{split} \psi_{n+2,m} + \psi_{n-2,m} + \psi_{n,m+2} + \psi_{n,m-2} - 4\psi_{n,m} \\ &= -\left(f_{n,m+1} + f_{n,m-1} + f_{n+1,m} + f_{n-1,m}\right) \\ &+ \left(E - 4\right)\left(\psi_{n,m+1} + \psi_{n,m-1} + \psi_{n+1,m} + \psi_{n-1,m}\right). \end{split}$$
(8)

Assuming that the potentials are randomly distributed, we introduce the smoothed wave function $\psi_{n,m}^{(2)}$ of the block and combine the terms $f_{n,m+1}+f_{n,m-1}+f_{n+1,m}+f_{n-1,m}$ to one single term $f_{n,m}^{(2)} \equiv \epsilon_{n,m}^{(2)} \psi_{n,m}^{(2)}$ with the block potential $\epsilon_{n,m}^{(2)} \equiv \epsilon_{n,m+1} + \epsilon_{n,m-1} + \epsilon_{n+1,m} + \epsilon_{n-1,m}$. Equation (8) now shows a block form of block length $\nu = 2$,



FIG. 2. Renormalization scheme for ν =4: the diagonal terms $f_{i,j} \equiv \epsilon_{i,j} \psi_{i,j}$ that form the block potential are painted black and show a chess-board pattern. The sites (n,m), (n+4,m), (n-4,m), (n,m+4), and (n,m-4) that couple via a Laplace operator of distance ν are symbolized by larger circles.

$$\psi_{n+1,m}^{(2)} + \psi_{n-1,m}^{(2)} + \psi_{n,m+1}^{(2)} + \psi_{n,m-1}^{(2)} - 4\psi_{n,m}^{(2)}$$
$$= -\epsilon_{n,m}^{(2)}\psi_{n,m}^{(2)} + 4(E-4)\psi_{n,m}^{(2)}.$$
(9)

This is shown in Fig. 1. Couplings between nearestneighbor sites via Eq. (1) are symbolized by straight lines whereas the couplings between the sites $\psi_{n+2,m}$ and $\psi_{n,m}$ and so on of Eq. (9) are symbolized by the oval lines. The site potentials $f_{n,m+i} \equiv \epsilon_{n,m+i}\psi_{n,m+i}$ and $f_{n+i,m} \equiv \epsilon_{n+i,m}\psi_{n+i,m}$ with $i=\pm 1$ that form the block potential $\epsilon_{n,m}^{(2)}$ are indicated by the black circles. It can be seen that they lie well inside an inclined block, consisting of 2² particles.

This procedure can be continued. By replacing again the site indices (n,m) of Eq. (9) by (n+1,m), (n-1,m), (n,m+1), and (n,m-1) and following the same procedure as before, we arrive at block indices $\nu=4$. As long as the block length is well below $\Lambda/2$, the Taylor expansion is legitimate and we arrive at higher and higher orders of the renormalization. The potential blocks form a chess-board pattern which is shown in Fig. 2 for the case of $\nu=4$. The renormalized Anderson equation of block length ν becomes

$$\psi_{n+1,m}^{(\nu)} + \psi_{n-1,m}^{(\nu)} + \psi_{n,m+1}^{(\nu)} + \psi_{n,m-1}^{(\nu)} - 4\psi_{n,m}^{(\nu)} = -\epsilon_{n,m}^{(\nu)}\psi_{n,m}^{(\nu)} + \nu^2(E-4)\psi_{n,m}^{(\nu)},$$
(10)

where $\psi_{n,m}^{(\nu)}$ is the smoothed wave function of a block of length ν and

$$\boldsymbol{\epsilon}_{n,m}^{(\nu)} \equiv \sum_{i^2 + j^2 < \nu^2, i + j \text{ odd}} \boldsymbol{\epsilon}_{i,j} \tag{11}$$

with the sum running over all pairs of *i* and *j* with *i* even, *j* odd and vice versa (chess-board pattern) in a distance $i^2 + j^2 < \nu^2$ from the site index (n,m).

III. THE SCALING ANSATZ: THEORY AND NUMERICAL SIMULATIONS

Now, the renormalization approach is complete and we use it to derive a scaling theory for the localization volume *V*. Naturally, the form of the wave function $\psi \sim \exp \times [-(r/\lambda)^{\Phi}]$ does not depend on the arbitrary subdivision of the lattice into blocks. Nevertheless, by applying the renormalization approach over a certain range of block lengths, we gain information about *V*.

The following derivation applies at E=4, where Λ diverges and the block form is legitimate for any block size between 1 and infinity. At E=4, the only quantities that enter into the right-hand side of Eq. (1) are the potentials $\epsilon_{i,j}$. Accordingly V, which is an average quantity over many lattice realizations, can only depend on the different moments of them (the first moment $\langle \epsilon \rangle$ being zero). As in d=1 we presume a power-law behavior,

$$V \sim \langle \epsilon^2 \rangle^{-\alpha}. \tag{12}$$

To derive the exponent α , we apply the block transformation described above separately to both sides of Eq. (12). The left-hand side, *V*, is a volume and therefore simply rescaled by a factor of ν^2 ,

$$V \to V_{\nu} \sim \frac{V}{\nu^2}.$$
 (13)

The right-hand side of Eq. (12) is determined by random walk theory. If we want to transform $\langle \epsilon^2 \rangle$ into $\langle \epsilon^2 \rangle_{\nu}$, we must first summarize over all ν^2 potentials $\epsilon_{i,j}$ of one block and then calculate the variance over many different blocks. This is equivalent to calculating the mean square displacement of a random walk of ν^2 steps,¹⁷

$$\langle \boldsymbol{\epsilon}^2 \rangle \rightarrow \langle \boldsymbol{\epsilon}^2 \rangle_{\nu} = \left\langle \left(\sum_{i=1}^{\nu^2} \boldsymbol{\epsilon}_i \right)^2 \right\rangle \sim \nu^2 \langle \boldsymbol{\epsilon}^2 \rangle.$$
 (14)

Transforming Eq. (12) by Eqs. (13) and (14) we find

$$\frac{V}{\nu^2} = \nu^{-2\alpha} \langle \epsilon^2 \rangle^{-\alpha}.$$
 (15)

As the last step, we must take into account that the block length ν is arbitrary for $\Lambda \rightarrow \infty$ and Eq. (15) must therefore not depend on ν . This determines the exponent α and we finally find

$$\alpha = 1$$
 and $V \sim \langle \epsilon^2 \rangle^{-1}$ for $E = 4$. (16)

In order to test Eq. (16), the eigenfunctions of systems of size 500×500 with varying variances $\langle \epsilon^2 \rangle$ have been calculated by the Lanczos algorithm. The different *V* have been determined using Eq. (3). For each $\langle \epsilon^2 \rangle$, we took the average over 40 systems and calculated the eigenfunctions in a small energy interval of $E=4\pm0.0002$. The results are shown in Fig. 3, where *V* is plotted versus $\langle \epsilon^2 \rangle$ in a double-logarithmic way. The line of slope -1/2 is a guide to the eye and represents the result of the scaling theory [see Eq. (16)]. Apart from slight finite-size effects for small $\langle \epsilon^2 \rangle$ (and therefore large $V^{1/2}$) it agrees very well with the numerical results.

The scaling theory can be extended to energies in some (small) distance from the band edge, where Λ is still large enough to perform the renormalization scheme over many steps. In Eq. (10), (4-E) is rescaled with ν^2 . Accordingly, we have [cf. Eqs. (13) and (14)]



FIG. 3. The effective localization length $V^{1/2}$ in the 2D Anderson model at the band edge is plotted versus the variance $\langle \epsilon^2 \rangle$ of the site potentials in a double-logarithmic plot. *V* was calculated numerically for lattices of size 500 × 500 with Dirichlet boundary conditions and averaged over 40 systems. The line of slope -1/2 is a guide to the eye and shows the theoretical behavior. Finite size effects occur for small values of $\langle \epsilon^2 \rangle$ (large values of $V^{1/2}$).

$$V_{\nu=1}((4-|E|),\langle\epsilon^2\rangle) \sim \nu^2 V_{\nu}(\nu^2(4-|E|),\nu^2\langle\epsilon^2\rangle).$$
(17)

Equation (17) is a generalized homogeneity relation. This means that the form of V remains unchanged when both, $\langle \epsilon^2 \rangle$ and 4-|E|, are rescaled according to the renormalization theory. Thus, V does not depend on both quantities separately, but only on a suitable combination of them.

The scaling form of V can now be derived by standard techniques. Choosing $\nu = \langle \epsilon^2 \rangle^{-1/2}$, (which is permitted for large $\langle \epsilon^2 \rangle$ even if Λ is not infinite) we find

$$V((4 - |E|), \langle \epsilon^2 \rangle) \sim \langle \epsilon^2 \rangle^{-1} g\left(\frac{4 - |E|}{\langle \epsilon^2 \rangle}\right)$$
(18)

with the scaling function g(x) and the argument

$$x = \frac{4 - |E|}{\langle \epsilon^2 \rangle}.$$
 (19)

For |E|=4, Eq. (18) must reduce to Eq. (16), yielding g(0)=1 for x=0. For small values of 4-|E| (large Λ) or large values of $\langle \epsilon^2 \rangle$ (small V), $\sqrt{V} \ll \Lambda$ and $x \ll 1$. In this case, the effective localization length \sqrt{V} is smaller than Λ , the system behaves as if Λ were infinite and g(x) should therefore be a constant function. For $x \ge 1$, the maximum block size becomes smaller and smaller, so that gradually, the scaling theory must break down. However, as in d=1, an intermediate range may exist, where g(x) still shows a power-law behavior.

In order to test Eq. (18), we have plotted $(V\langle\epsilon^2\rangle)^{1/2}$ as a function of $(4-E)/\langle\epsilon^2\rangle$ for different disorder widths w of the potentials, $\epsilon_i \in [-w/2, w/2]$ with $\langle\epsilon^2\rangle = w^2/12$ and for different values of 4-E. The numerical simulations were again carried out on 500×500 lattices and the average was performed over 40 systems and in an energy interval



FIG. 4. As a test of Eq. (18), $(V\langle\epsilon^2\rangle)^{1/2}$ is plotted versus the argument $x \equiv (4-E)/\langle\epsilon^2\rangle$ for different disorder widths w=0.6 (circles), w=0.8 (squares), w=1.0 (diamonds), w=1.2 (triangles up), and w=1.5 (triangles down) with $\langle\epsilon^2\rangle = w^2/12$ and for different values for 4-E between 0.001 and 0.06. The average was again taken over 40 systems of size 500×500 .

[4-E-0.0002, 4-E+0.0002] for different values of 4-Ebetween 0.001 and 0.06. With decreasing values of $\langle \epsilon^2 \rangle$, *V* increases and finite size effects occur. Additionally, systems where $\langle \epsilon^2 \rangle$ and (4-E) are both small or both large, possess large error bars, i.e., large fluctuations between different values of *V*. In the case of small $\langle \epsilon^2 \rangle$, this also gives rise to finite size effects, because some very large values of *V* are suppressed by the finite system size. So, we restrict ourselves to not too large values of 4-E and to combinations, where such large fluctuations do not occur.

The results are shown in Fig. 4 and confirm the scaling ansatz (18) very well. Different symbols that indicate different $\langle \epsilon^2 \rangle$ fall onto the same universal curve. We can see that indeed g(x) reaches a plateau, $g(x) \approx \text{const}$ for small values of x where V is simply described by Eq. (16) (see above). For large values $x \gg 1$, on the other hand, the scaling theory must break down, possibly after an intermediate range with a different power-law behavior of g(x). It would be very interesting to investigate also this regime, However, large values of x have not been calculated, because—due to the increasing values of \sqrt{V} —we needed much larger system sizes for the simulations. This is currently not possible.

IV. CONCLUDING REMARKS

In summary, a renormalization scheme has been developed close to the band edges (i.e., in the limit of large wavelengths) that analytically reduces the Anderson equations (1) into block form where the block sizes may become arbitrarily large at the band edges. A Taylor expansion consistent with the standard interpretation of the Anderson equations has been used. A scaling form for the localization volume V has been derived from this. Contrary to former renormalization schemes,^{18,19} it does not involve successive recalculations of the matrix elements in each step, but simply replaces Eq. (1) by Eq. (10), where the off-diagonal elements are unchanged and the diagonal elements of arbitrary block size ν are directly related to the diagonal elements of the original system. The works of Refs. 18 and 19 proposed the mobility edge in d=3 and scaling laws for the conductivity and related quantities. Therefore, it will be very interesting to extend also the present theory to the three-dimensional Anderson model. However, as it is developed for energies close to the band edge it is for the moment not clear, if it can be applied to the vicinity of the mobility edge, where comparisions to former renormalization theories can be made.

As a last remark, we would like to note that the regime $x \ge 1$ is also relevant to the vibrational problem with unit spring constants and fluctuating masses $m_{n,m} = \langle m \rangle + \tilde{m}_{n,m}$, where $\langle m \rangle$ describes the average mass and $\tilde{m}_{n,m}$ the disorder of them. If we transform Eq. (1) according to

$$4 - E \to \langle m \rangle \omega^2, \epsilon_{n,m} \to \widetilde{m}_{n,m} \omega^2$$
(20)

with the eigenfrequency ω of the vibration, we find the vibrational equation

$$\frac{1}{m_{n,m_{n',m'}}} \sum_{m',m'} (\psi_{n',m'} - \psi_{n,m}) = -\omega^2 \psi_{n,m}, \qquad (21)$$

with the sum going over all neighbors of the site (n,m). Inserting the above transformation into Eq. (5), we find for the wavelength in the vibrational case $\Lambda \ge (\langle m \rangle^{1/2} \omega)^{-1}$. The limit of long wavelengths applies thus for $\omega^2 < 1/\langle m \rangle$. Positive masses lead to $\langle \tilde{m}^2 \rangle < \langle m \rangle^2$ and together with Eq. (19) we finally arrive at x > 1.

So, in the vibrational case, only the branch of higher values of the scaling variable x exists and it will be very interesting to investigate also this part. However, since this demands much larger system sizes (due to the increasing values of V), this should be done in the future.

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