

Inverse Participation Ratio in $2 + \varepsilon$ Dimensions*

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The averaged moments of the eigenfunctions (including the inverse participation ratio) of a particle in a random potential are considered near the mobility edge. The exponents of the power laws are given in an ε -expansion in one-loop order for a $d = 2 + \varepsilon$ dimensional system. The calculation is based on a recent formulation of the mobility edge problem which maps it onto a model of interacting matrices.

1. Introduction and Results

Several criteria have been given (see for example [1]) to distinguish the energy regions of extended and localized states of a quantum mechanic particle in a random potential. One criterion is the d.c. conductivity which vanishes in the region of the localized states but is positive for the energies of the extended states. Another criterion is the inverse participation ratio which averages the fourth power of the wavefunction. It is positive for localized states and vanishes for extended states in the thermodynamic limit.

Here the critical behaviour of the averaged powers of the following quantities are considered as a function of energy E near the mobility edge E_c :

- (i) of the wavefunction in the region of the localized states

$$P^{(k)}(E) = \overline{\sum_i |\psi_i(r)|^{2k} \delta(E - e_i)} / \rho(E) \sim (E_c - E)^{\pi_k} \quad (1.1)$$

and

- (ii) of the average of the squared wavefunction within an energy width η in the region of the extended states

$$\begin{aligned} 1/p^{(k)}(E) &= \lim_{\eta \rightarrow 0} \overline{[\sum_i |\psi_i(r)|^2 \delta_\eta(E - e_i)]^k} / \rho^k(E) \\ &\sim (E - E_c)^{-\mu_k} \end{aligned} \quad (1.2)$$

with the Lorentzian

$$\delta_\eta(x) = \frac{\eta/\pi}{\eta^2 + x^2} = \frac{1}{2\pi i} \left(\frac{1}{x - i\eta} - \frac{1}{x + i\eta} \right). \quad (1.3)$$

Here $\psi_i(r)$ is the amplitude of the eigenfunction $|i\rangle$ with energy e_i at site r of the particle in a tight-binding model. $\rho(E)$ is the density of states per site and energy. $P^{(2)}$ is the inverse participation ratio. For $k > 1$ the quantity $P^{(k)}$ vanishes in the region of the extended states and $p^{(k)}$ vanishes for localized states. For a tight-binding model with real matrix elements an ε expansion for a $d = 2 + \varepsilon$ dimensional system predicts

$$\mu_k = k(k-1) + O(\varepsilon), \quad (1.4)$$

$$\pi_k = (k-1)(2\varepsilon^{-1} + 1 - k) + O(\varepsilon). \quad (1.5)$$

The exponents μ_k and π_k are related by

$$\pi_k = (k-1)dv - \mu_k \quad (1.6)$$

where v is the exponent for the localization length.

The calculation is based on a recent formulation [2] of the mobility edge problem which expresses the averaged Green's functions as correlations of components of interacting matrices Q . Their critical behaviour is examined by means of renormalization group techniques.

In Sect. 2 the participation ratio and related quantities are discussed and connected to the averaged

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Green's functions. The scaling behaviour of these functions is derived in Sect. 3. The derivation of the exponents $x = -\mu/\nu$ is explained in Sect. 4.

2. Inverse Participation Ratio and Related Quantities

Bell and Dean [3] (compare [4]) have introduced the concept of a partition ratio \hat{p}_i for an eigenstate $|i\rangle$ of a disordered system. If the wavefunction $\psi_i(r)$ at sites r of a tight-binding model is normalized then \hat{p}_i is given by

$$\hat{p}_i = 1/(N \sum_r |\psi_i(r)|^4) \quad (2.1)$$

where N is the number of lattice sites. Besides \hat{p}_i the "inverse participation ratio" P_i has been defined as (compare [1])

$$P_i = \sum_r |\psi_i(r)|^4. \quad (2.2)$$

(Note that P_i is not the inverse of \hat{p}_i but $\hat{p}_i P_i = 1/N$). The meaning of these quantities becomes apparent by a simple example. Suppose the wavefunction spreads over l lattice sites with equal amplitude $|\psi_i(r)|^2 = 1/l$ and vanishes elsewhere. Then one has

$$\hat{p}_i = l/N, \quad P_i = 1/l. \quad (2.3)$$

Thus \hat{p}_i describes the proportion of the total number of atoms in a system which contribute effectively to an eigenstate, whereas P_i is the inverse number of orbitals contributing effectively to this state. For localized (normalizable states) P_i is larger than zero whereas \hat{p}_i vanishes in the thermodynamic limit $N \rightarrow \infty$. If the eigenstate is concentrated in one orbital then P_i attains its maximum value unity. For a plane wave, $\psi_i(r) = e^{iq_i r}/\sqrt{N}$, \hat{p}_i assumes its maximum value $\hat{p}_i = 1$ whereas P_i vanishes in the thermodynamic limit $N \rightarrow \infty$. Quite generally P_i vanishes for extended states. Probably \hat{p}_i is positive for these states. However, this is not proven. (Compare a discussion of various possibilities by Last and Thouless [5].)

Instead considering P_i for individual eigenstates of individual systems one introduces the ensemble averaged quantity

$$P^{(2)}(E) = \overline{\sum_{i,r} |\psi_i(r)|^4 \delta(E - e_i)} / \overline{\sum_i \delta(E - e_i)} \quad (2.4)$$

(the bar indicates the ensemble average). The denominator is given by the density ρ of states per site and energy

$$\overline{\sum_i \delta(E - e_i)} = N \rho(E). \quad (2.5)$$

If the average

$$\overline{\sum_i |\psi_i(r)|^4 \delta(E - e_i)}$$

does not depend on r then P can be written

$$P^{(2)}(E) \rho(E) = \overline{\sum_i |\psi_i(r)|^4 \delta(E - e_i)}. \quad (2.6)$$

In order to determine P we use that the two-particle spectral function

$$S_2(E_1, E_2) = \overline{\langle r | \delta(E_1 - H) | r \rangle \langle r | \delta(E_2 - H) | r \rangle} \quad (2.7)$$

contains a δ -function contribution

$$\overline{\sum_i |\psi_i(r)|^4 \delta(E_1 - e_i) \delta(E_2 - E_2)}, \quad (2.8)$$

so that the limit

$$P^{(2)}(E) \rho(E) = 2\pi \lim_{\eta \rightarrow 0} (\eta A_2(\eta, E)) \quad (2.9)$$

with

$$\begin{aligned} A_2(\eta, E) &= \int \delta_\eta(E - E_1) \delta_\eta(E - E_2) S_2(E_1, E_2) dE_1 dE_2 \\ &= (-4\pi^2)^{-1} \left(\langle r | \frac{1}{E - i\eta - H} - \frac{1}{E + i\eta - H} | r \rangle \right)^2 \end{aligned} \quad (2.10)$$

extracts the $|\psi_i(r)|^4$ contributions. Economou and Cohen [6] have used this quantity to define localization. Thus $P^{(2)}(E)$ can be obtained from the knowledge of the two-particle Green's functions which enter A_2 , (2.10).

The situation is more difficult for \hat{p} which cannot be extracted from the continuum of states entering $A_2(\eta, E)$ in such an obvious way. Therefore we introduce a quantity $p^{(2)}$, instead, which is obtained by replacing $|\psi_i(r)|^2$ by an average of $|\psi(r)|^2$ over an energy width η and taking the limit $\eta \rightarrow 0$.

$$\begin{aligned} 1/p^{(2)}(E) &= \lim_{\eta \rightarrow 0} \lim_{N \rightarrow \infty} \{ N^2 \overline{[\sum_i |\psi_i(r)|^2 \delta_\eta(E - e_i)]^2} / \\ &\quad \overline{(\sum_i \delta_\eta(E - e_i))^2} \} \end{aligned} \quad (2.11)$$

so that

$$\rho^2(E)/p^{(2)}(E) = \lim_{\eta \rightarrow 0} A_2(\eta, E). \quad (2.12)$$

From the calculation for an n -orbital model [7] we expect that $p^{(2)}$ has a finite limit for $\eta \rightarrow 0$ in the region of extended states.

Obviously $P^{(2)}(E)$ and $p^{(2)}(E)$ can be generalized to $P^{(k)}$ and $p^{(k)}$ as defined in the introduction. In order to determine $P^{(k)}$ we observe that the k -particle spectral function

$$S_k(E_1, \dots, E_k) = \overline{\prod_{j=1}^k \langle r | \delta(E_j - H) | r \rangle} \quad (2.13)$$

contains a δ -function contribution

$$\sum_i |\psi_i(r)|^{2k} \prod_{j=1}^k \delta(E_j - e_i). \quad (2.14)$$

With

$$C_k = \eta^{k-1} \int_{-\infty}^{+\infty} (\delta_\eta(x))^k dx = (2\pi)^{1-k} \frac{(2k-3)!!}{(k-1)!} \quad (2.15)$$

and

$$A_k(\eta, E) = \left(\frac{1}{2\pi i} \right)^k \overline{\left\langle r \left| \frac{1}{E - i\eta - H} - \frac{1}{E + i\eta - H} \right| r \right\rangle^k} \quad (2.16)$$

one obtains

$$P^{(k)}(E) \rho(E) = C_k^{-1} \lim_{\eta \rightarrow 0} (\eta^{k-1} A_k(\eta, E)). \quad (2.17)$$

Similarly to $p^{(2)}$, Eq. (2.12), one finds

$$\rho^k(E)/p^{(k)}(E) = \lim_{\eta \rightarrow 0} A_k(\eta, E), \quad (2.18)$$

so that the determination of $P^{(k)}$ and $p^{(k)}$ is reduced to that of k -particle Green's functions at the same site r .

3. Scaling Behaviour

Now the formulation of [2] is used which allows us to represent the averaged two-particle Green's functions

$$K = -4\pi^2 \overline{\langle r | \delta_\eta(E-H) | r' \rangle \langle r' | \delta_\eta(E-H) | r \rangle} \quad (3.1)$$

$$K'' = -4\pi^2 \overline{\langle r | \delta_\eta(E-H) | r \rangle \langle r' | \delta_\eta(E-H) | r' \rangle} \quad (3.2)$$

with the partial fraction decomposition of δ_η , Eq. (1.3), in terms of averages over products of matrices Q

$$K = \sum_{pp'} (-)^{p+p'} \langle Q_{ab}^{pp'}(r) Q_{ba}^{p'p}(r') \rangle, \quad a \neq b \quad (3.3)$$

$$K'' = \sum_{pp'} (-)^{p+p'} \langle Q_{aa}^{pp}(r) Q_{bb}^{p'p'}(r') \rangle, \quad a \neq b \quad (3.4)$$

where p and p' run over 1 and 2.

These averages have to be evaluated for a Hamiltonian

$$\mathcal{H} = \frac{1}{4} \hat{K} \int d^d r \operatorname{tr} (\nabla Q(r) \nabla Q(r)) + \frac{1}{4} \eta \nu^{-1} \int d^d r \sum_{p,a} (-)^p Q_{aa}^{pp}(r). \quad (3.5)$$

The symmetric matrices Q have two eigenvalues λ_1

and λ_2 of multiplicities $m_1 = m_2 = 0$ where λ_1 and λ_2 are the averaged one-particle Green's functions

$$\lambda_{1,2} = \overline{\langle r | \frac{1}{E \mp i\eta - H} | r \rangle}. \quad (3.6)$$

The first term of \mathcal{H} is invariant under orthogonal transformations of Q , the second one breaks this symmetry, but vanishes for $\eta \rightarrow 0$.

For $r=r'$ the expressions (3.1) and (3.2) coincide. However, it is not obvious that (3.3) and (3.4) are equal for $r=r'$. Indeed the formulation in terms of the composite variables Q is only valid in the gauge-invariant limit, that is, on a length scale large in comparison to the phase coherence length (the mean free path). Therefore in order to obtain the mobility edge behaviour of A_2 , Eq. (2.10), we will consider local operators which have the same symmetry as those entering (3.3) and (3.4) with $r=r'$. The operators in (3.3) and (3.4) can be written

$$O_4 = \sum_{ijkl} v_{ijkl} Q_{ij}(r) Q_{kl}(r) \quad (3.7)$$

where index pairs (p, a) are abbreviated by one index i . Since the matrices Q are symmetric we require

$$v_{ijkl} = v_{jikl} = v_{klij}. \quad (3.8)$$

Apparently the coefficients of v for the operators O_4 entering (3.3) and (3.4) obey

$$\sum_i v_{iikl} = \sum_i v_{ijil} = 0. \quad (3.9)$$

This property tells us that the operators O_4 transform under orthogonal transformations of the Q 's like components of an angular momentum with $l=4$. Since for $\eta \rightarrow 0$ the Hamiltonian (3.5) is invariant under orthogonal transformations only operators with $l=4$ must be considered.

There are two irreducible representation of these operators, a symmetric one with

$$v_{ijkl} = v_{ikjl} = v_{ilkj} \quad (3.10)$$

and an asymmetric one with

$$v_{ijkl} + v_{ikjl} + v_{ilkj} = 0 \quad (3.11)$$

(The dimension of these representations with respect to permutations of the indices is 1 and 2, resp.) A one-loop calculation for these operators yields the following exponents x

$$x_{2s} = -2\varepsilon + O(\varepsilon^2), \quad x_{2a} = \varepsilon + O(\varepsilon^2) \quad (3.12)$$

where $y=d-x$ is the full dimension of the operator. The full dimension of the symmetric operator exceeds

the space dimensionality. This is unusual for conventional critical phenomena where all operators obey $x \geq 0$, $y \leq d$. Here it reflects the strong fluctuations of the wavefunctions in the region of extended states near the mobility edge.

There are also operators cubic in Q and of higher orders in Q with $l=4$. Since Q has only two eigenvalues they can be reduced to expressions bilinear in Q . There are also operators with spacial derivatives. Their dimension is smaller by one or several integers. Therefore they yield only corrections to the leading scaling behaviour.

In order to discuss the mobility edge behaviour we recall that under a renormalization group step which changes the length scale by a factor b the operator O , $E-E_c$, and the "frequency" η are multiplied by b^x , $b^{1/\nu}$, and b^d resp. [7-9]. Thus the expectation value of O can be written

$$\langle O \rangle = (E - E_c)^{x\nu} f(\eta / (E - E_c)^{d\nu}). \quad (3.13)$$

Since both K and K'' contain a contribution from the symmetric operator and since $x_{2s} < x_{2a}$, the symmetric one yields the dominant contribution with

$$x_{2s}\nu = -2 + O(\varepsilon) \quad (3.14)$$

since [2]

$$\nu = 1/\varepsilon + O(\varepsilon). \quad (3.15)$$

In the region of the extended states one expects that the limit

$$\lim_{\eta \rightarrow 0} A_2(\eta, E) \sim \langle O \rangle = (E - E_c)^{x\nu} \lim_{\eta \rightarrow 0} f(\eta / (E - E_c)^{d\nu}) \quad (3.16)$$

is finite. Therefore with (3.15) one obtains that $p^{(2)}(E)$ decays like

$$p^{(2)}(E) \sim (E - E_c)^{\mu_2} \quad (3.17)$$

with

$$\mu_2 = -x_{2s}\nu = 2 + O(\varepsilon). \quad (3.18)$$

In the region of the localized states one expects, compare (2.9),

$$\begin{aligned} & \lim_{\eta \rightarrow 0} (\eta A_2(\eta, E)) \\ & \sim (E - E_c)^{x_{2s}\nu + d\nu} \lim_{\eta \rightarrow 0} \frac{\eta}{(E - E_c)^{d\nu}} f\left(\frac{\eta}{(E - E_c)^{d\nu}}\right) \end{aligned} \quad (3.19)$$

to be finite. Thus $P^{(2)}(E)$ obeys for $E \leq E_c$ the power law

$$P^{(2)}(E) \sim (E_c - E)^{\pi_2} \quad (3.20)$$

with

$$\pi_2 = (x_{2s} + d)\nu = 2\varepsilon^{-1} - 1 + O(\varepsilon). \quad (3.21)$$

The exponent κ' in [8] is identical with $-x_{2s}$.

The mobility edge behaviour of A_k , Eq. (2.16), for $k=3, 4, 5, \dots$ can be obtained in a similar way. It is expressed as expectation value of a homogeneous polynomial of order k in Q , which belongs to the representations of angular momentum $l=2k$. For $k=3$ there are three irreducible representations, a symmetric one with

$$x_{3s} = -6\varepsilon + O(\varepsilon^2) \quad (3.22)$$

and two other representations

$$x_{3a} = -\varepsilon + O(\varepsilon^2), \quad x_{3b} = 3\varepsilon + O(\varepsilon^2). \quad (3.23)$$

The dimension of these representations with respect to the permutations of the indices is 1, 9, and 5 resp. The exponent x of the symmetric representation is for all k the lowest one yielding the most singular contribution

$$x_{k,s} = -k(k-1)\varepsilon + O(\varepsilon^2). \quad (3.24)$$

Following the same arguments as for $k=2$ one obtains

$$\mu_k = -x_{k,s}\nu \quad (3.25)$$

and (1.4) to (1.6).

If it is allowed to extrapolate (3.24) to non-integer k , then the exponent κ in [8] obeys $\kappa = 2x_{1/2,s} = \varepsilon/2 + O(\varepsilon^2)$.

4. Remarks on the One-Loop Calculation

In one-loop order the exponents x_s (and ν) can be obtained by the following argument: The diagrams for the model (3.5) for matrices Q with two eigenvalues of multiplicity m_1 and m_2 in one-loop order have combinatorial factors linear in m_1 and m_2 , however the model is invariant under exchange of m_1 and m_2 [10]. Thus the one-loop result depends only on $m_1 + m_2$. Furthermore the n -vector model is a special case of this matrix model with components

$$Q_{ij} = S_i S_j, \quad (4.1)$$

and $m_1 = 1$ eigenvalue S^2 and $m_2 = n - 1$ eigenvalues zero [10]. Thus we take the $(2+\varepsilon)$ expansion for the nonlinear σ -model, put $n = m_1 + m_2 = 0$ and obtain immediately ν from the known solution [11, 12]. The substitution of (4.1) in our k th order polynomials in Q yields $(2k)$ th order polynomials in S for the

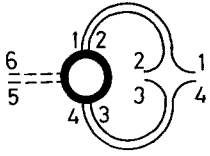


Fig. 1. One-loop diagram to Γ

symmetric operators, but zero for all asymmetric ones. Thus in one-loop order we use the result of [13] and obtain

$$x_{k,s} = -\zeta_{2k}(n=0) = -k(k-1)\varepsilon + O(\varepsilon^2). \quad (4.2)$$

The exponents of the antisymmetric operators are obtained in the following way. The diagram which determines the critical exponent of the irreducible vertex function Γ_k , that is the exponent $x_k - kx_1$ (for arbitrary multiplicities of m_1 and m_2) in one-loop order has the form shown in Fig. 1. The black ring indicates the insertion. For $k=2$ the diagram is valid without the broken lines, for $k=3$ the broken lines have to be added. The propagators are shown as double lines carrying both indices. The insertion is of the form $Q_{12}Q_{34}$ and $Q_{12}Q_{34}Q_{56}$, resp. Apparently the insertion $Q_{12}Q_{34}$ generates a contribution to $(Q_{14}Q_{23})$ and upon exchange of 3 and 4 a contribution to $(Q_{13}Q_{24})$. In order to obtain x one has to diagonalize the matrix cM with three entrances for the products $Q_{12}Q_{34}$, $Q_{13}Q_{24}$, $Q_{14}Q_{23}$ where c is some constant and

$$M = \begin{pmatrix} 0 & 1 & 1 \\ 1 & 0 & 1 \\ 1 & 1 & 0 \end{pmatrix}. \quad (4.3)$$

The eigenvectors are $(1, 1, 1)$, $(1, -1, 0)$, $(0, 1, -1)$ with eigenvalues $a=2, -1, -1$ resp. They correspond to the symmetric and asymmetric operators (3.10) and (3.11). Since $x_1=0$ for $m_1=m_2=0$ and since $x_{2s} = -2\varepsilon$ we have $c = -\varepsilon$ and thus

$$x = -\varepsilon a + O(\varepsilon^2). \quad (4.4)$$

For $k>2$ we use group theory. For general k we obtain from $Q_{12}Q_{34}Q_{56} \dots Q_{2k-1,2k}$ altogether $q = (2k-1)!!$ different products by permuting the $2k$ indices. The permutations applied on these q products Q define a representation D of the symmetric group. The operator M which produces out of a given insertion of type Q^k the one-loop contributions to Γ_k can be constructed from the operator

$$C = \sum_{i>j} (ij) \quad (4.5)$$

which is the sum of all transpositions. If (ij) is one of

the k pairs $(1, 2), (3, 4), \dots, (2k-1, 2k)$ then it reproduces the product $Q_{12}Q_{34} \dots Q_{2k-1,2k}$. All other contributions to C exchange two indices of two factors Q . For example (13) and (24) generate $Q_{14}Q_{32}Q_{56} \dots Q_{2k-1,2k}$. In total one finds

$$C = k + 2M. \quad (4.6)$$

The eigenvalues of C are obtained in the following way: The representation D of the symmetric group reduces to several irreducible representations. Each representation has a certain eigenvalue to C . It is given by the character χ_2 of the class of transpositions, that is the class of permutations $(2, 1^{2k-2})$. This character has to be multiplied by the total number of transpositions

$$g_2 = k(2k-1), \quad (4.7)$$

since C is the sum of all of them, and finally to be divided by the order χ_0 of the representation, since χ_2 is the trace over the representation. χ_0 itself is the character of the identical transformation, the class being denoted by (1^{2k}) . Thus the eigenvalues of C are

$$\xi = g_2 \chi_2 / \chi_0, \quad (4.8)$$

and the eigenvalues of M are

$$a = (\xi - k)/2. \quad (4.9)$$

The representations of the symmetric group are characterized by partitions of the number $2k$ into positive integers $\lambda_1, \lambda_2, \dots, \lambda_m$ with

$$\lambda_1 \geq \lambda_2 \geq \dots \geq \lambda_m \quad (4.10)$$

and

$$\sum_{i=1}^m \lambda_i = 2k. \quad (4.11)$$

The quantity a can be calculated from the formula for ξ in the book by Hamermesh [14],

$$a = \sum_{i=1}^m \frac{\lambda_i}{2} \left(\frac{\lambda_i}{2} - i \right). \quad (4.12)$$

There remains the question: Which partitions are contained in the representation D ? We cannot answer this question. However, for $k=1, 2, 3$ D contains precisely the representations for which all λ_i are even. For $k=4, 5$ it turns out that

$$\sum \chi_0 a^n = \text{tr}(M^n)$$

holds for $n=0, 1, 2, 3$ where the sum runs over all representations with even λ 's. The corresponding par-

Table 1. χ_0 and a for partitions with even λ 's

k	Partition	χ_0	a
1	(2)	1	0
2	(4)	1	2
	(2 ²)	2	-1
3	(6)	1	6
	(4, 2)	9	1
	(2 ³)	5	-3
4	(8)	1	12
	(6, 2)	20	5
	(4 ²)	14	2
	(4, 2 ²)	56	-1
	(2 ⁴)	14	-6
5	(10)	1	20
	(8, 2)	35	11
	(6, 4)	90	6
	(6, 2 ²)	225	3
	(4 ² , 2)	252	0
	(4, 2 ³)	300	-4
	(2 ⁵)	42	-10

tions and χ_0 , a are listed in Table 1. Thus it seems likely that D contains the representations character-

ized by partitions for which all λ 's are even precisely once and no other representations.

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