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THE ONE-DIMENSIONAL ANDERSON MODEL: ANOMALY IN THE BAND CENTRE

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Weak disorder expansion of the Lyapunov exponent γ of an electron in the one-dimensional Anderson model with a diagonal and off-diagonal disorder is presented. The band centre anomaly of expansion is analysed: For $E = 0$ the anomalous behaviour of γ and of all its even moments is found. For the diagonal disorder, the true values of γ and of the density of states are calculated. For the system with the off-diagonal disorder, we find for $E = 0$ an infinite localization length and prove the divergency of all even moments of γ.

1. INTRODUCTION

The problem of the band-centre anomaly of the Lyapunov exponent $\gamma(E)$ in the one-dimensional ($1D$) Anderson model is of interest since the numerical work of Czychol et al. [1]. They found that for a system with a diagonal disorder (DD) the nondegenerate weak disorder expansion (WDE) of LE, proposed by Thouless [2] does not work in the neighbourhood of $E = 0$ (band centre). This discrepancy has been explained by several authors, and the true value of LE has been found in [3—6]. It has been shown that in the neighbourhood of $E = 0$ γ depends only on the disorder λ and on the ratio $x = E/\lambda^2$. The anomalies of the same origin appear also in the quasi-one-dimensional systems [7, 8] and for the $1D$ system with the off-diagonal disorder (ODD) [9—18].

Recently [9] we have proposed a new method of the calculation of LE, based on the supersymmetric representation of the Green function. This treatment enables us to find the WDE of LE for systems with both DD and ODD. In the neighbourhood of $E = 0$, however, we obtained only a $1/x$-expansion of $\gamma(x)$. To find $\gamma(x)$ for all values of x one needs information about the behaviour of γ for $x \to 0$. Its derivation presents the main aim of this paper.

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The paper is organized as follows: In § 2 we propose the simple method of calculation of WDE of LE for DD. Our method is similar to that of Lambert [5]. We find the 2nd order term of $\gamma(E)$ for $E \neq 0$. In § 3, the true value of $\gamma(x = 0)$ is calculated. It is shown that the band-centre anomaly is present also in the E-dependence of all even moments of γ. For ODD, we find for $E \neq 0$ the WDE up to the 2nd order in disorder (§ 4). For $E = 0$, we obtain $\mathrm{Re}\,\gamma(E = 0) = 0$ in agreement with the results published previously [10—16]. The calculation of the higher moments of $\sigma = \gamma - i\pi/2$ confirms that all even moments of σ diverge as $E \to 0$.

2. THE WEAK DISORDER EXPANSION-DIAGONAL DISORDER

We start with the Hamiltonian

$$H = \sum_n \{|n+1\rangle\langle n| + |n\rangle\langle n+1|\} + \lambda \sum_n e_n |n\rangle\langle n| \tag{1}$$

where e_n are random independent energies with zero mean value. From (1) the set of equations for the wave function in the sites n can be written

$$\Psi_{n-1}(E) + (\lambda e_n - E)\,\Psi_n(E) + \Psi_{n+1}(E) = 0. \tag{2}$$

The Lyapunov exponent is defined as [4]

$$\gamma(E) = \langle \log(\Psi_{n+1}/\Psi_n)\rangle = \lim_{N\to\infty} N^{-1} \sum_n \log[\Psi_{n+1}/\Psi_n]. \tag{3}$$

From γ the density of states can be found as [4]

$$\varrho(E) = -\frac{\partial\, \mathrm{Im}\,\gamma(E)}{\pi\,\partial E}. \tag{4}$$

For $\lambda = 0$ eqs. (2) have the trivial solution

$$\Psi_n(E) = t^{-n} = \exp(iqn),$$

where the energy $E = 2\cdot\cos q$, and $t = \exp(-iq)$.

For $\lambda \neq 0$ we substitute the Ansatz

$$\Psi_n(E) = t^{-n}\cdot\exp(\xi_n), \tag{5}$$

then (2) can be rewritten into the reccurent formula

$$\sigma_{n+1} = \log[1 + t^2(1 - \exp(-\sigma_n)) - t\lambda e_n], \tag{6}$$

where $\sigma_{n+1} = \xi_{n+1} - \xi_n = \gamma_{n+1} - iq$.

For $E \neq 0$ one can expand the right-hand-side of (6) into the power series in λ, σ_n. Supposing $\langle \sigma_n^4\rangle \sim \lambda^4$, and keeping only the terms proportional to λ^2, we obtain

$$\sigma_{n+1} = -t\lambda e_n - \lambda^2 t^2 e_n^2/2 + \sigma_n t^2 - \sigma_n^2 t^2(1+t^2)/2. \quad (7)$$

Averaging (7) gives

$$\sigma(1-t^2) = -at^2/2 - \sigma_2 t^2(1+t^2)/2, \quad (8a)$$

where $\sigma_2 = \langle \sigma_n^2 \rangle$, $\sigma = \langle \sigma_n \rangle$, $a = \lambda^2 \langle e^2 \rangle$.

Squaring both sides of (7) and averaging gives

$$\sigma_2(1-t^4) = at^2. \quad (8b)$$

From (8a, b) one obtains

$$\sigma = -\frac{a}{2}\frac{t^2}{(1-t^2)^2} = -\frac{a}{8(1-E^2/4)}, \quad (9)$$

i.e. the result of Thouless [2].

3. THE BAND-CENTRE ANOMALY

As $E \to 0$, eq. (8b) gives the singularity of σ_2; to study this situation more properly, let us substitute

Then

$$E = ax. \quad (10)$$

$$t = -\mathrm{i}(1+az), \qquad z = \mathrm{i}x/2,$$

which transforms (7) into

$$\sigma_{n+1} = -\sigma_n + \log[1 - 2az(\exp(\sigma_n) - 1) + \mathrm{i}(1+az)\lambda e_n \cdot \exp(\sigma_n)]; \quad (11)$$

expanding the right-hand side of (11) into the power series in λ, and keeping all terms proportional to λ^2, we obtain

$$\sigma_{n+1} = -\sigma_n - 2az[\exp(\sigma_n) - 1] + \mathrm{i}\lambda e_n \cdot \exp(\sigma_n) + a \cdot \exp(2\sigma_n)/2 + 0(\lambda^3). \quad (12)$$

Expanding the right-hand side of (12) into the k-th power and everaging the resulting equations, we obtain the following set of equations:

$$\sigma = \frac{\lambda^2\langle e^2\rangle}{4}\left\{1 + \sum_{m=2}^{\infty}\frac{1}{m!}\sigma_m(2^m - 4z)\right\} \quad (12.1)$$

where $\sigma_m = \langle \sigma_n^m \rangle$, $\sigma_0 = 1$, $\sigma_1 = \sigma$, and

$$\sigma_m\{1 - (-1)^m - a\cdot(-1)^m\cdot(2mz - m^2)\} =$$

$$= a(-1)^m\left\{-\frac{m(m-1)}{2}\sigma_{m-2} - \frac{m(2m-1)}{2}\sigma_{m-1}\right\} + a/2\sum_{k=1}^{\infty}\sigma_{m+k}\left\{\frac{4mz}{(k+1)!} - \frac{2^{k+1}}{(k+2)!}m\cdot(k+2m)\right\} \qquad m = 2, 3, \ldots \quad (12m)$$

The most important consequence of eqs. (12) is the fact that near the band centre all σ_{2m} behave as λ^0. Indeed, eq. (12.2) gives

$$\sigma_2(4-4z)\cdot a \sim a\cdot[-1+\ldots]$$

so that

$$\sigma_2 \sim \frac{1}{4(z-1)}.$$

Similarly, eq. $(4\cdot 2m)$ gives

$$4\cdot(m^2 - mz)\cdot a\cdot\sigma_{2m} \sim -\sigma_{2(m-1)}\cdot a\cdot m(2m-1) + \ldots$$

and so $\sigma_{2m} \sim \lambda^0$ too. For the odd moments we obtain $\sigma_{2m+1} \sim \lambda^2$, hence their behaviour is "normal".

From this point of view, eq. (12.1) gives an explanation of the anomaly of γ near the band centre: to receive γ up to the 2nd order in λ, we have to calculate all even moments σ_{2m} up to the order zero.

Omitting all odd terms (proportional to λ^2), we rewrite the system (12m) into the form

$$\sigma_{2m}(4m^2 - 4mz) = -m(2m-1)\sigma_{2m-2} + 4\sum_{k=1}^{\infty}\sigma_{2m+2k}\left\{\frac{mz}{(2k+1)!} - \frac{2^{2k}}{(2k+2)!}\cdot m(k+2m)\right\}. \quad (13m)$$

Taking

$$\sigma_{2m} = \alpha_m + \beta_m\cdot z, \qquad m = 0, 1, 2, \ldots \quad (14)$$

we obtain two systems of linear equations

$$\bar{A}\alpha = -\delta_{i1}$$
$$\bar{A}\beta = \bar{B}\alpha. \quad (15m)$$

The form of the matrices $\bar{A}$, $\bar{B}$ is evident from eqs. (13). The solve the systems (15) we have to choose the number of equations we take into account. In Table 1 we present the values of $\mathrm{Re}\,\gamma$ and of the density of states (4) calculated for systems with 1—10 equations. Quick convergence to the value is given both by the factorial in the denominators in eq. (12.1), and by the quick decreasing of σ_{2m}, which is evident from Table 2.

Table 1

Re γ and density of states calculated from system (15) using the first n equations

n	Re γ	$2\pi \cdot \varrho(0)$
1	0.125000	1.
2	.115385	1.012204
3	.114362	1.014660
4	.114250	1.015025
5	.114238	1.015073
6	.114237	1.015079
7	.114237	1.015080
10	.114237	1.015080

Table 2

The first 10 even moments of σ calculated from eqs. (15) using 14 equations (in approximation $\sigma_{30} = 0$)

m	α_m	β_m
1	−0.317735	−0.427681
2	.148466	.300065
3	−0.076701	−0.189805
4	.041524	.116965
5	−0.023099	−0.071418
6	.013080	.043450
7	−0.007500	−0.026397
8	.004341	.016031
9	−0.002531	−0.009736
10	.001484	.005915

4. OFF-DIAGONAL DISORDER

The method presented in §§ 2, 3 may be applied also to the system with *ODD*. Now the Hamiltonian reads

$$H = \sum_n \beta_{n+1} \{|n+1\rangle\langle n| + |n\rangle\langle n+1|\}, \tag{16}$$

where $\beta_n = 1 + \Lambda v_n$, and v_n are the random independent variables. For simplicity we suppose the probability distribution $P(v_n)$ such that $P(|v_n| > 1/\Lambda) = 0$.

The equations for the vawe function now read

$$\beta_{n+1} \Psi_{n+1} - E\Psi_n + \beta_n \Psi_{n-1} = 0. \tag{17}$$

Using (5) we obtain

$$\sigma_{n+1} + \log \beta_{n+1} = \log\{1 + t^2[1 - \exp(-\sigma_n)] - t^2 \cdot \Lambda \cdot v_n \exp(-\sigma_n)\}. \tag{18}$$

Apart from the term $\log \beta_{n+1}$ on the left-hand side, the exponential factor $\exp(-\sigma_n)$ in the last term makes the only difference between eqs. (6) and (18). For energies far from the band centre we expand (18) as

$$\sigma_{n+1} + \Lambda v_{n+1} - \Lambda^2 v_{n+1}^2/2 = t^2\sigma_n - t^2(1+t^2)\sigma_n^2/2 - t^2\Lambda v_n - - \Lambda^2 v_n^2/2 \cdot t^4 + \Lambda t^2(1+t^2)\sigma_n v_n. \tag{19}$$

Averaging (19) we obtain

$$\sigma(1 - t^2) = \frac{b}{2}(1 - t^4) - \frac{t^2}{2}(1 + t^2)\sigma_2 - \Lambda t^2(1 + t^2)\langle\sigma_n v_n\rangle \tag{20}$$

with $b = \Lambda^2\langle v^2\rangle$. Multiplying (19) by v_{n+1} and averaging gets

$$\Lambda\langle\sigma_{n+1} v_{n+1}\rangle = -b. \tag{21}$$

Finally, for σ_2 we obtain from (19)

$$\sigma_2(1 - t^4) = (1 + t^4)b - 2t^4\Lambda\langle\sigma_n v_n\rangle. \tag{22}$$

The system (20)—(22) has the solution

$$\sigma_2 = \frac{1 + 3t^4}{1 - t^4} b \tag{23}$$

$$\sigma = \frac{1 - 4t^2 - t^4}{2(1 - t^2)^2} b. \tag{24}$$

Eq. (24) is equivalent to the formula (45) from [9].

From (23) we see that for $E \to 0$ ($t \to -\mathrm{i}$) σ_2 again diverges, and so relation (24) holds only for energies far from the band centre. For

$$E = bx \tag{25}$$

we have

$$t = -\mathrm{i}(1 + bz) \tag{26}$$

and from (23) we obtain the leading term of σ_2

$$\sigma_2 \sim z^{-1}. \tag{27}$$

Thus, as well as in the *DD*-case, $\sigma_2 \sim b^0$.

Substitution of (25), (26) into (19) gives

$$\sigma_{n+1} + \log \beta_{n+1} = -\sigma_n + \log[\beta_n - 2bz[\exp(\sigma_n) - 1]] \tag{28}$$

from which we obtain

$$\sigma = -bz[\langle\exp\sigma_n\rangle - 1], \tag{29}$$

$$z \cdot \langle\sigma_n \cdot \exp\sigma_n\rangle = 1 + 0(b). \tag{30}$$

Thus, $\langle \sigma_n \cdot \exp(\sigma_n) \rangle$ diverges as $z \to 0$, and we cannot construct the system of equations similar to that for DD.

Substituting $z = 0$ in (28) we find directly

$$\sigma_{n+1} + \log \beta_{n+1} = -\sigma_n + \log \beta_n \tag{31}$$

so that

$$\sigma(z = 0) = 0 \tag{32}$$

for any disorder, as referred to also in (10)—(15).

Squaring and averaging of (31) gives

$$\langle \sigma_{n+1}^2 \rangle - \langle \sigma_n^2 \rangle = 4 \cdot \{\langle \log^2 \beta \rangle - \langle \log \beta \rangle^2\}, \tag{33}$$

where we used the identity

$$\langle \sigma_n \log \beta_n \rangle = -\langle \log^2 \beta_n \rangle + \langle \log \beta_n \rangle^2. \tag{34}$$

From (33) we have

$$\langle \sigma_n^2 \rangle \sim 4n \quad \text{for} \quad z = 0. \tag{35}$$

In this way we can find similar anomalies for all $\langle \sigma_n^{2m} \rangle (z = 0)$. Moreover, from (18) we find

$$\langle \exp(\sigma_n) \rangle \sim \left[\langle \beta_n^2 \rangle \cdot \left\langle \frac{1}{\beta_n^2} \right\rangle \right]^n \tag{36}$$

as $\langle \beta_n^{-1} \rangle > \langle \beta_n \rangle = 1$, $\langle \exp \sigma_n \rangle$ grows exponentialy with n.

5. CONCLUSION

We presented the WDE of the Lyapunov exponent of the electron in the one-dimensional Anderson model with both a diagonal and an off-diagonal disorder. In the neighbourhood of the band centre, we analysed the anomaly of LE γ: for the case with the diagonal disorder we derived the system of linear equations for γ and for its higher even moments. The system can be easily solved giving the true value of $\gamma(0)$. As all even moments of σ proceed to the non-zero limit independent of the disorder in the band centre and in the limit of weak (but non-zero) disorder, we conclude that for $E = 0$ the probability distribution of $\mathrm{Re}\,\gamma$ does not converge to the δ-function as $\lambda \to 0$, but keeps the finite width.

For the case of ODD, we confirm the well-known result that the mean value of $\mathrm{Re}\,\gamma$ approaches zero as $E \to 0$. Our method is, however, not suitable for deriving the E-dependence of γ in the neighbourhood of $E = 0$. It is due to the non-analyticity of $\gamma(E)$ near $E = 0$ [16, 17]. The calculation of the higher moments of σ proves the divergency of all even moments of σ for $E = 0$. Thus we argue together with [17, 18] that in spite of the infinite localization length the electron is always localized due to the large fluctuations of $\mathrm{Re}\,\gamma$.

Anomalies, similar to the band-centre anomaly, discussed in this paper, arise also in the generalized one-dimensional Anderson model [19], and in any quasi-one-dimensional Anderson model [8]. In the last case there are, besides the anomalies $q = \pi/2$, also the anomalies of expansion in the neighbourhood of the energies caused by the so-called accidental degeneracy [8]. It can be shown [8, 19, 20] that in the neighbourhood of the corresponding "critical" energy E_c the LE are functions only of λ and $x = (E - E_c)/\lambda^2$. We hope that for the cases where $\gamma(x)$ is an analytical function of x, we can generalize the method presented in this paper, and find the "true" values of all the corresponding LE.

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ОДНОМЕРНАЯ МОДЕЛЬ АНДЕРСОНА: АНОМАЛИЯ В ЦЕНТРЕ ЗОНЫ

Для одномерной модели Андерсона с диагональным и недиагональным беспорядком найдено разложение экспоненты Ляпунова (ЭЛ) в степенях беспорядка. Предложен анализ особенности разложения в центре зоны: для $E = 0$ найдены аномалии ЭЛ и всех его четных моментов. Для диагонального беспорядка найдены настоящие значения ЭЛ и плотности состояний. Для системы с недиагональным беспорядком получены для $E = 0$ бесконечная длина локализации и расходимость всех четных моментов ЭЛ.