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Transport regimes and critical energies in the two-dimensional Anderson model

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Abstract. We calculate numerically the energy level distributions of the two-dimensional Anderson model in the nearly clean, ballistic, diffusive and strongly localized regimes. The Poisson statistics governs nearest level spacings in the clean (in the absence of degeneracies due to the geometry) and localized regimes, whereas in the ballistic and diffusive regimes the level statistics follows the Wigner–Dyson distribution. In the diffusive and ballistic regimes, we study the critical energy E_c, defined as the maximum energy up to which level fluctuations follow the logarithmic behaviour characteristic of random-matrix theory (RMT). A reasonably accurate determination of the ballistic–diffusive transition is achieved through the behaviour of the critical energies. We show how the level statistic is an adequate tool for characterizing the different regimes of disordered systems, and how the results obtained are in qualitative agreement with theoretical estimates. We finally analyse the behaviour of E_c as a function of the energy within the band.

1. Introduction

Scaling theory [1] of Anderson localization suggests that there exists no conducting state in an infinite two-dimensional disordered system at zero temperature, since all one-electron wave functions are localized even for arbitrarily small fluctuations of a random potential. The corresponding energy levels are distributed completely at random. Therefore, for any non-vanishing disorder the distribution of nearest level spacings is given by the Poisson law in the thermodynamic limit. For finite systems, we have different regimes according to the ratio between the different length scales and the linear size of the system (or alternatively in terms of the ratio between energy scales). For a fixed linear size L ($L < l_\phi$, where l_ϕ is the phase-breaking length) we can classify the systems into four regimes, which in order of decreasing disorder are:

(i) *the strongly localized regime*: when the Anderson localization length ξ is smaller than L ($L > \xi$);

(ii) *the diffusive regime*: when the localization length is larger than L but the elastic mean free path l is smaller than L ($l < L < \xi$);

(iii) *the ballistic regime*: when the elastic mean free path l is larger than L, and the mixing of the crystal states by the disorder potential is larger than the level spacing ($1 < lL^{-1} < p_F L$, where p_F is the Fermi momentum); and

(iv) *the clean limit*: when the energy perturbation of each state is smaller than the mean level spacing Δ ($lL^{-1} > p_F L$).

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Our aim is to investigate this classification using the level statistics of the corresponding systems. The study of level statistics of disordered quantum systems has attracted considerable attention recently. In particular, the spectral correlations of these systems play a fundamental role in the study of quantum chaos and in the physics of mesoscopic systems.

There are several quantities that measure the fluctuations of energy levels. In the RMT they depend only on the symmetry of the Hamiltonian. If it is invariant under rotations and under time-reversal symmetry, the fluctuations are described by the Gaussian orthogonal ensemble (GOE) of random matrices [2–4]. There is a repulsion between nearest levels, whose spacings follow Wigner–Dyson statistics [3, 5–7]. This is true for diffusive as well as for ballistic systems, provided that the typical value of the disorder energy exceeds the mean level spacing, which implies that the energy spectra differ drastically from the clean case. Two of these quantities widely used in literature are the following.

(i) The distribution $P(s) = \langle \delta(\epsilon - \epsilon_i + \epsilon_{i+1}) \rangle$ of the normalized spacing $s = \epsilon/\Delta$ between consecutive levels. In the GOE it is well described by the Wigner surmise

$$P_{\mathrm{W}}(s) = \frac{\pi s}{2} \exp\left(-\frac{\pi s^2}{4}\right) \tag{1}$$

while, when there is no correlation between levels, it has a Poissonian behaviour:

$$P_{\mathrm{P}}(s) = \exp(-s). \tag{2}$$

(ii) The number variance $\Sigma^2(E)$:

$$\Sigma^2(E) = \langle \delta N^2(E) \rangle = \langle N^2(E) \rangle - \langle N(E) \rangle^2. \tag{3}$$

This measures the fluctuation in the number of levels $N(E)$ in a strip of width E. The average $\langle\ \rangle$ can be taken either over several realizations of disorder or, as usual in quantum chaos, over different regions of the spectrum. For the uncorrelated case, the number variance is Poisson like:

$$\Sigma^2_{\mathrm{P}}(E) = E \tag{4}$$

while for the GOE, $\Sigma^2(E)$ increases logarithmically with E [3, 7]:

$$\Sigma^2_{\mathrm{W}}(E) \approx \frac{2}{\pi^2}\left[\ln(2\pi E) + \gamma + 1 - \frac{\pi^2}{8}\right] \tag{5}$$

where $\gamma = 0.5772\ldots$ is Euler's constant. Note that for sufficiently large E the dependence of Σ^2 on E is much weaker than the linear dependence expected for uncorrelated energy levels. Long-range fluctuations of the GOE are thus very small, a characteristic known as spectral rigidity.

Levels follow a Poisson distribution only if the disorder W is strong enough that the localization length ξ is shorter than the system size L. With decreasing W the electron states change gradually from strongly localized to weakly localized and the energy levels become more correlated. When $\xi > L$ their statistics is well described by the Wigner–Dyson distribution. The number variance of the spectra of quantum Hamiltonians obeying Wigner–Dyson statistics follows the GOE behaviour up to a critical energy, generically known as the Thouless energy [8]. We will use this critical energy to investigate the ballistic–diffusive transition.

In this paper we carry out a numerical analysis of the energy spectra of the 2D Anderson model. We vary the disorder energy W for a given linear size L in order to obtain the four above-mentioned regimes. Through $P(s)$ we study the frontier between strongly localized

and diffusive systems, on one hand, and between ballistic and nearly clean systems on the other hand. The analysis of the critical energy and fluctuations above it allows us to distinguish between diffusive and ballistic systems.

2. The model and numerical procedures

The dynamics of non-interacting electrons in the presence of disorder that breaks the translational symmetry can be investigated using the tight-binding Hamiltonian

$$H = \sum_{\boldsymbol{r}} \omega_{\boldsymbol{r}} |\boldsymbol{r}\rangle\langle\boldsymbol{r}| + \sum_{\langle \boldsymbol{r} \neq \boldsymbol{r}' \rangle} t_{\boldsymbol{r}\boldsymbol{r}'} |\boldsymbol{r}\rangle\langle\boldsymbol{r}'| \tag{6}$$

where the vectors $\boldsymbol{r}$ label the sites of the sample, and the $t_{\boldsymbol{r}\boldsymbol{r}'}$ are the non-diagonal transfer matrix elements connecting sites $\boldsymbol{r}$ and $\boldsymbol{r}'$ (the symbol $\langle\ \rangle$ restricts the sum to nearest-neighbour sites). The uncorrelated random energies $\omega_{\boldsymbol{r}}$ are distributed with constant probability within the interval $(-W/2, W/2)$, where W denotes the strength of the disorder. We will consider square samples of size $L \times L$, and with a lattice constant a. In the following we take $t_{\boldsymbol{r}\boldsymbol{r}'} \equiv t = -1$ and $a = 1$, which set up the energy unit and length unit, respectively. Calculations have been carried out on samples of sizes up to $L = 60$, and, for each value of the disorder W, we consider at least 1000 different realizations. In computing the whole spectrum we used the Schwarz algorithm for symmetric band matrices [9].

In order to characterize the statistical properties of the spectra it is customary to map each real spectrum $\{\epsilon_i\}$ onto the unfolded spectrum $\{E_i\}$ through $E_i = \overline{N}(\epsilon_i)$, where $N(\epsilon_i)$ is the number of levels up to an energy ϵ_i, and the overline denotes averaging over different disorder realizations. The spectrum $\{E_i\}$ has on the average a constant mean spacing equal to one. After rescaling, the number variance in an energy window $[\epsilon_{\mathrm{F}}, \epsilon_{\mathrm{F}} + E]$ is calculated, where the initial energy is called ϵ_{F} by analogy with the Fermi energy, since this is the relevant energy in the calculations of some magnitudes. In this work, Σ^2 has been obtained by a different numerical procedure [10] which gives a better account of the fine details of the number variance. We have checked that the overall features are procedure independent, i.e. that our method coincides with the standard one when subtleties are ignored.

The method, which gives no fluctuations in the clean limit, has the following features. For each value of W and L an energy window around ϵ_{F} is defined: $[\epsilon_{\mathrm{F}} - \delta/2, \epsilon_{\mathrm{F}} + \delta/2]$. Random energies ϵ_1 and ϵ_2 within this interval are chosen. The mean number of levels within interval $[\epsilon_1, \epsilon_2]$ is given by

$$\overline{N} = \langle N(\epsilon_1) - N(\epsilon_2) \rangle_W \tag{7}$$

where $N(\epsilon)$ gives the total number of states below energy ϵ for a particular disorder realization; $\langle\ \rangle_W$ indicates averaging over disorder configurations. In the same way, the mean of the squared number of levels in this energy interval is given by

$$\overline{N^2} = \langle [N(\epsilon_1) - N(\epsilon_2)]^2 \rangle_W . \tag{8}$$

The variance of the number of levels contained in the energy interval $[\epsilon_1, \epsilon_2]$ is simply

$$\Sigma^2(\overline{N}) = \overline{N^2} - \overline{N}^{\,2} . \tag{9}$$

This provides a value of $\Sigma^2(\epsilon_{\mathrm{F}}, E)$ (note that $E = \overline{N}$). The sequence is repeated a large number of times for randomly selected energy intervals $[\epsilon_1, \epsilon_2]$ within $[\epsilon_{\mathrm{F}} - \delta/2, \epsilon_{\mathrm{F}} + \delta/2]$ until a relatively smooth value is obtained for the variance of the number of levels *averaged* over energy intervals containing the same number of levels. The last step implies averaging over the selected energy region around ϵ_{F}.

3. Level spacing distributions

We first try to obtain as much information as possible from the nearest level spacing distributions. In the strongly localized regime the level spacing follows a Poisson distribution since localized states are usually spaced far apart, and so their energies are not correlated. On the other hand, diffusive and ballistic systems have overlapping wave functions with strong correlations which produce a Wigner–Dyson distribution of level spacings. In the nearly clean limit (in 2D) we obtain again Poisson statistics, because the energy of each level corresponds to a sum of two uncorrelated contributions, each one associated with a component of the quasi-momentum.

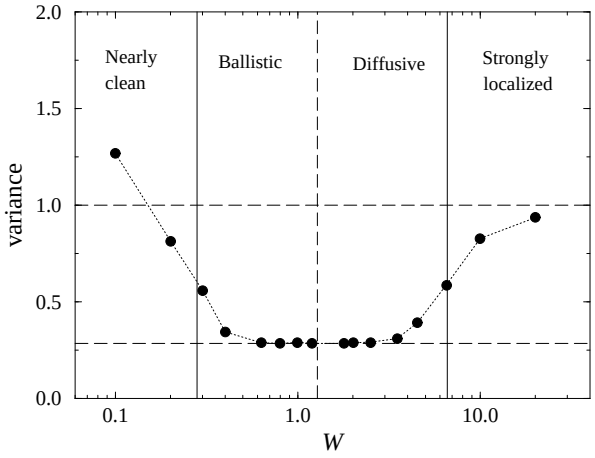

Figure 1. The variance of the nearest level spacing distributions as a function of the disorder parameter W for a system with $L = 50$. The results correspond to an average over an energy window $(-2.2, -1.8)$. The dashed horizontal lines correspond to the Poisson (1) and Wigner (0.286) variances. The vertical solid lines mark the clean–ballistic and diffusive–localized transitions. The vertical dashed line corresponds to the ballistic–diffusive transition.

A suitable way to study a transition from a Poisson to a Wigner distribution is through the variance of s, namely, $\langle s^2 \rangle - \langle s \rangle^2$. This variance is equal to 1 and 0.286 for a Poisson and for a Wigner–Dyson distribution, respectively. In figure 1 we show on a logarithmic scale the variance of the nearest level spacing distribution $P(s)$ as a function of the disorder parameter W for the system size $L = 50$. The horizontal lines correspond to the Poisson and Wigner–Dyson variances. As expected we can clearly see two transitions: one from a Poisson to a Wigner distribution, corresponding to the change from the clean limit to the ballistic regime, and another from a Wigner to a Poisson distribution, corresponding to the diffusive-to-localized transition. We have marked with vertical solid lines both transitions, which we now analyse separately. The vertical dashed line represents the ballistic–diffusive transition, which is not reflected in the behaviour of the variance, and which will be studied in the next section.

3.1. Transitions from clean to ballistic systems

The critical disorder for the clean–ballistic transition is approximately that for which the spreading width induced by the disorder perturbation is equal to the mean level spacing. As the site disorder energies are uncorrelated, the previous spreading width is equal to the

standard deviation of the disorder energy of a single site divided by the square root of the number of sites. In our case this is equal to $\sigma = W/(\sqrt{3}L)$. As the average level spacing is $8/L^2$, the critical disorder is given by

$$W_c = \frac{8\sqrt{3}}{L}. \tag{10}$$

For the size corresponding to the figure, $L = 50$, equation (10) predicts a value of 0.28. This critical disorder is indicated in figure 1 by means of a vertical line which lies in the region where the variance is changing from the value corresponding to the Wigner–Dyson distribution (0.286) to that of the Poisson distribution (see figure 1). Note that for very low disorder strengths the variance is greater than 1. This deviation between the value found numerically and the corresponding value of the Poisson distribution is due to degeneracies caused by the square geometry [11].

3.2. Transitions from diffusive to strongly localized systems

We estimate the critical disorder for the diffusive–localized transition from the condition $\xi = L$, ξ being the localization length, where $L = 50$ for the data reported in figure 1. Using the results of references [12, 13] we can obtain the disorder parameter W corresponding to this localization length. In order to do so we have to take into account the fact that we are not studying the centre of the band ($\epsilon = 0$) whose states become most delocalized since the kinetic energy is maximal for tight-binding models, but an energy $\epsilon = -2$ [14]. W turns out to be approximately 6.6. This value is indicated in figure 1 by means of a vertical line which again lies in the region where the variance is changing from the Wigner–Dyson to the Poisson value. Similar results are obtained for $L = 20$ and $L = 40$. Note that the critical disorder for the transition from the diffusive to the strongly localized regime only depends weakly on L [12–14].

4. The critical energy

As we remarked in the introduction, disordered systems with extended states can be either diffusive or ballistic depending on whether the elastic mean free path l is smaller or larger than the linear size of the system L, respectively. The mean free path l can be obtained from the imaginary part of the self-energy, $l = v_F\tau_F = \hbar v_F/2|\mathrm{Im}\,\Sigma(\epsilon_F)|$. From this expression, l can be written in terms of the model's parameters as [15, 16]

$$l \approx 6\hbar v_F/(W^2\pi\nu(\epsilon_F)). \tag{11}$$

The spectra of these systems always obey Wigner–Dyson statistics, but exhibit different types of long-range (in energy) fluctuations depending on whether they are diffusive or ballistic. In this section we try to find the ballistic–diffusive transition through the study of long-range fluctuations of the energy levels, or more specifically through the number variance $\Sigma^2(\epsilon_F, E)$ and the critical energies.

In figure 2 we show, on a double-logarithmic scale, $\Sigma^2(\epsilon_F, E)$ as a function of the normalized energy E for the 2D Anderson model with $L = 50$, $\epsilon_F = -2$ and different values of the disorder strength. The thin lines give the linear and logarithmic behaviour of the Poisson and GOE, respectively. The uppermost curve corresponds to the strongly localized regime ($W = 20$) and follows the Poisson behaviour quite well, as expected. The next curve ($W = 2$) gives the fluctuations of a diffusive case, for which the ratio l/L is approximately 0.2. Fluctuations follow the GOE up to a critical energy and then increase

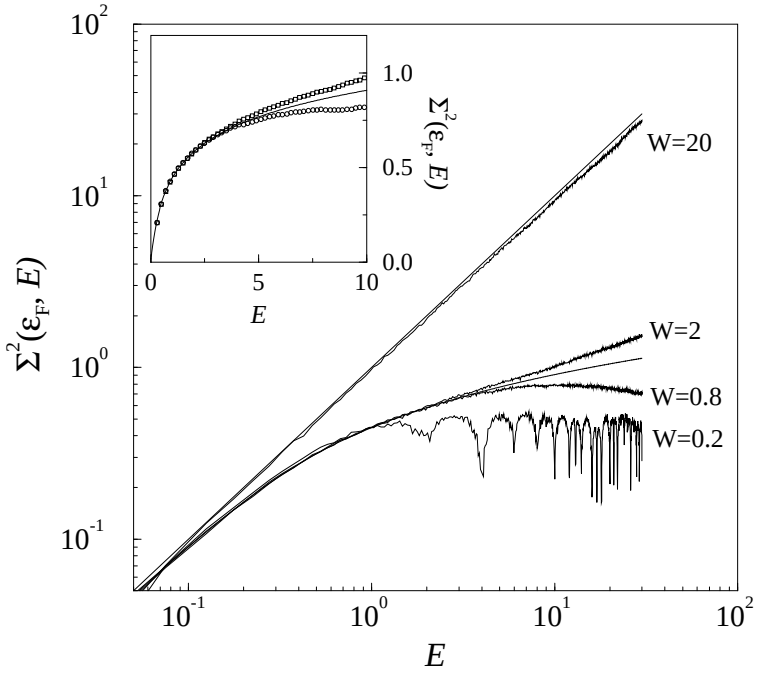

Figure 2. $\Sigma^2(\epsilon_F, E)$ as a function of E for $L = 50$ and $\epsilon_F = -2$. The thin lines give the Poisson (upper) and Wigner fluctuations (lower). The inset shows the corresponding values for the diffusive (squares) and ballistic (circles) regimes on normal scales.

beyond the GOE, although at a much slower pace than in the completely uncorrelated case. The second curve from the bottom corresponds to the ballistic regime ($W = 0.8$ and $l/L \approx 1.34$). A critical energy which sets a limit on the applicability of RMT also exists in this regime. For energies higher than the critical one, the fluctuations are smaller than predicted by the GOE and remain almost constant as soon as they deviate from the logarithmic behaviour. The lowest curve ($W = 0.2$) gives the fluctuations in the nearly clean regime. We can note that these fluctuations are small, and oscillate as a function of energy as a consequence of finite-size oscillations in the density of states [17].

In the inset of figure 2, we show $\Sigma^2(\epsilon_F, E)$ for the diffusive (squares) and ballistic (circles) regimes on normal scales. The thin line represents the result for the GOE. In determining E_c we have used curves similar to these ones for different values of L and W. The criterion that we have followed is that E_c is the energy at which the numerical results for the fluctuations deviate by 2% from the GOE.

A direct way to obtain the critical disorder strength for the diffusive–ballistic transition is by finding the value whose fluctuations follow those of the GOE as closely as possible. However, in practice, it is more convenient to find the transition from the behaviour of the critical energy, as we do now. The critical energy in the diffusive regime (the Thouless energy) is associated with the inverse transport time through the system, and in normalized units is given by [16]

$$E_c^D = \frac{3\hbar^2 v_F^2}{\pi} W^{-2} \tag{12}$$

where v_F is the Fermi velocity. In ballistic systems, the critical energy loses its meaning as an inverse transport time through the system, and in normalized units is equal to [16, 18]

$$E_c^B = \frac{L^2 \pi \nu^2(\epsilon_F)}{6} W^2. \tag{13}$$

While the critical energy increases with disorder as W^2 in the ballistic regime, it decreases as W^{-2} in the diffusive case. We will use this fact to estimate the critical disorder of the ballistic–diffusive transition. In the numerical calculations we have taken $\hbar = 1$.

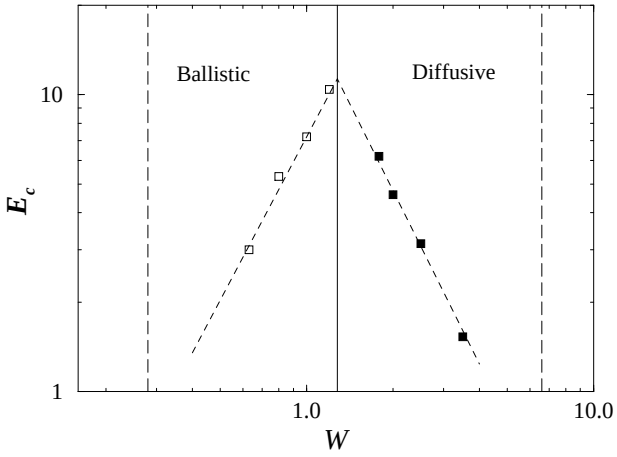

Figure 3. A log–log plot of the critical energy E_c in the ballistic (open squares) and diffusive (filled squares) regimes as a function of the disorder parameter W for $L = 50$ and an energy average over the range $(-2.2, -1.8)$. The fitted straight lines are: $E_c^B = (7.4 \pm 1.0) W^{(1.88 \pm 0.14)}$ (ballistic); and $E_c^D = (19.8 \pm 1.0) W^{(-2.04 \pm 0.08)}$ (diffusive). The vertical dashed lines mark the clean–ballistic and diffusive–localized transitions. The solid line corresponds to the ballistic–diffusive transition.

In figure 3 we show on a log–log scale the critical energy E_c in the ballistic (open squares) and diffusive (filled squares) regimes as functions of the disorder parameter W for $L = 50$. The results are averaged over an energy range $(-2.2, -1.8)$. The fitted straight lines are: $E_c^B = (7.4 \pm 1.0) W^{(1.88 \pm 0.14)}$ (ballistic); and $E_c^D = (19.8 \pm 1.0) W^{(-2.04 \pm 0.08)}$ (diffusive). The slopes of the two straight lines, -2.04 and 1.88, are in good agreement with the theoretical predictions of the exponents of W, -2 and 2, from equations (12) and (13), respectively. The numerical results for the factor multiplying the power of W do, however, disagree with the results obtained from equations (12) and (13). In the ballistic regime equation (13) gives 13.1, to be compared with the numerical result 7.4. The disagreement is even more important in the diffusive regime—namely, whereas equation (12) gives 4.8, our numerical result is 19.8.

The dashed lines mark the clean–ballistic and diffusive–localized transitions obtained in the previous section. The solid line represents the ballistic–diffusive transition and goes through the crossing point of the two straight lines fitting the critical energies in the two regimes.

The critical disorder energy for this transition can be estimated by equating the two critical energies, equations (12) and (13). We arrive at

$$W_c = \sqrt{\frac{2^{1/2}3\hbar v_F}{\pi \nu}} L^{-1/2}. \tag{14}$$

W_c for this transition decreases with increasing system size L at a slower pace than for the clean–ballistic transition but at a faster pace than for the diffusive–localized transition. For the size considered in the figure ($L = 50$) equation (14) predicts a value of 0.8, not far from the numerical result (1.28) obtained from the results for the critical energies shown in figure 3. The mean free path corresponding to the numerical result for the critical disorder is 26, which is of the order of the actual system size ($L = 50$).

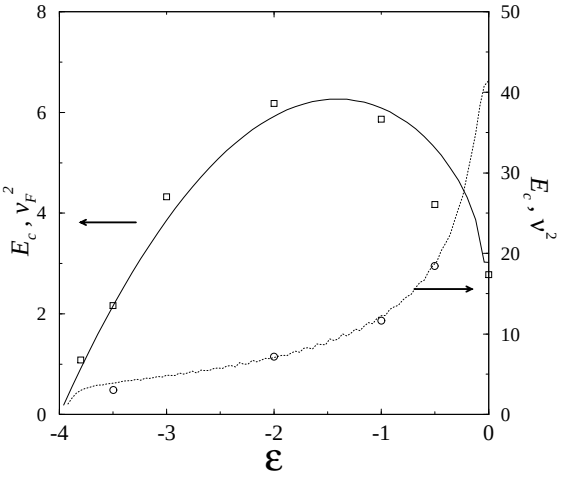

Figure 4. The critical energy E_c as a function of energy in the diffusive, $W = 1.8$ (squares) and ballistic, $W = 1.0$ (circles) regimes. It was calculated by averaging for each energy ϵ in the range $(\epsilon - 0.2, \epsilon + 0.2)$. The solid line is a fit to E_c in the diffusive case, proportional to v_F^2, and the dashed line is a fit to the results of the ballistic case, proportional to $\nu^2(\epsilon_F)$.

In order to complete the study of the critical energy we have calculated E_c as a function of the initial energy ϵ_F. In figure 4 we plot these results for $L = 50$ and two values of the disorder, $W = 1.8$ in the diffusive regime (squares) and $W = 1.0$ in the ballistic regime (circles). We also plot the square of the Fermi velocity (solid line), fitted by using a constant factor to the results of the diffusive case, and the square of the density of states (dotted line), fitted by using a different factor to the results of the ballistic case. We observe significant variations in E_c which reproduce changes in the Fermi velocity (diffusive case; equation (12)) and in the density of states (ballistic regime; equation (13)). The proportionality constant in the ballistic case is 740, approximately a factor of two smaller than the theoretical value of equation (13), namely 1309. For the diffusive case, this factor is 1.24, about four times the theoretical prediction, namely 0.3.

5. Conclusions

We have performed a systematic numerical analysis of energy fluctuations in the 2D Anderson model, over a wide range of parameters, in the nearly clean, ballistic, diffusive

and strongly localized regimes. Averages were taken over different realizations of disorder. The main conclusions of our study are as follows.

(i) The nearest level spacing distribution is appropriate for determining the critical disorder for the transition from the nearly clean to the ballistic require and for the transition from the diffusive to the strongly localized regime.

(ii) In the ballistic and diffusive regimes, the fluctuations follow those of the GOE up to a critical energy E_c above which the behaviour of such systems is different.

(iii) We determine the ballistic–diffusive transition from the behaviour of E_c.

(iv) The numerical results obtained for E_c qualitatively reproduce the expected behaviour—namely, it is proportional to W^{-2} and to W^2 in the diffusive and ballistic regimes, respectively.

(v) We checked that E_c is also proportional to the square of the Fermi velocity (the diffusive case) and to the square of the density of states (the ballistic regime).

Summarizing, the level statistics of disordered systems is a very valuable tool for characterizing the different transport regimes of these systems.

Acknowledgments

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References

[1] Abrahams E, Anderson P W, Licciardello D C and Ramakrishnan T V 1979 *Phys. Rev. Lett.* **42** 673
[2] Efetov K B 1983 *Adv. Phys.* **32** 53
Bohigas O, Giannoni M J and Schmit C 1984 *Phys. Rev. Lett.* **52** 1
Akkermans E and Montambaux G 1992 *Phys. Rev. Lett.* **68** 642
[3] Brody T A, Flores J, French J B, Mello P A, Pandey A and Wong S S M 1981 *Rev. Mod. Phys.* **53** 385
[4] Al'tshuler B L and Shklovskii B I 1986 *Zh. Eksp. Teor. Fiz.* **91** 220 (Engl. Transl. 1986 *Sov. Phys.–JETP* **64** 127)
[5] Gutzwiller M C 1990 *Chaos in Classical and Quantum Mechanics* (New York: Springer)
[6] Bohigas O 1991 *Proc. Les Houches Summer School (1989)* ed M-J Giannoni, A Voros and J Zinn-Justin (New York: Elsevier) Session L11
[7] Mehta M L 1991 *Random Matrices* (San Diego, CA: Academic)
[8] Thouless D J 1977 *Phys. Rev. Lett.* **39** 1167
[9] Schwarz H R 1968 *Numer. Math.* **12** 231
[10] Louis E, Cuevas E, Vergés J A and Ortuño M 1996 *Phys. Rev.* B **56** 2120
[11] Casati G, Chirikov B V and Guarneri I 1985 *Phys. Rev. Lett.* **54** 1350
[12] MacKinnon A and Kramer B 1983 *Z. Phys.* B **53** 1
[13] Zharekeshev Kh, Batsch M and Kramer B 1996 *Europhys. Lett.* **34** 587
[14] Sheng P 1995 *Introduction to Wave Scattering, Localization, and Mesoscopic Systems* (San Diego, CA: Academic)
[15] Economou E N 1983 *Green's Functions in Quantum Physics* (Berlin: Springer)
[16] Cuevas E, Louis E, Ortuño M and Vergés J A 1998 *Phys. Rev.* B at press
[17] Gasparian V, Louis E and Vergés J A 1996 *Phys. Rev.* B **53** 6967
[18] Altland A, Gefen Y and Montambaux G 1996 *Phys. Rev. Lett.* **76** 1130