LOCALIZATION TRAJECTORY AND CRITICAL INDEX

Isa Kh. Zharekeshev
Al-Farabi Kazakh National University, Almaty

Electron localization in chaotic systems is studied by using the method of transfer-matrices. The critical index of the localization length is found.

Introduction

A phenomenon of localization of a quantum particle by a random impurity potential has been a very intriguing subject for several past decades and is still one of present active research. After formulating the problem by Anderson, developing a field-theoretical formalism by Wegner followed by the renormalization group analysis in $2 + \varepsilon$ dimensions and, finally, introducing the hypothesis of the one-parameter scaling major properties of the localization length in disordered systems have been established. One of the central ideas is that for arbitrary small randomness, electron wave functions can be either localized or extended, depending on the number of dimensions. Basically the scaling theory [1] predicts a discontinuous transition from extended to localized states for any spatial dimension exceeding two ($d > 2$).

This disorder-driven transition between metallic and insulating phases can be described by a typical set of parameters characteristic of a critical phenomenon, in analogy with conventional quantum phase transitions known from statistical mechanics. For example, the correlation length of the transition asymptotically diverges as a power law with the critical exponent ν. According to the nonlinear σ-model the exponent is solely defined by the dimensionality and the fundamental symmetry irrespective of microscopic details (potential distribution, lattice structure, type of disorder, anisotropy etc.).

Although substantial progress in the understanding of critical behaviour at the disorder-induced metal insulator transition has been achieved, nevertheless several issues are still considered as being open and unsolved. Among them are effects of boundary conditions and the validity of one-parameter scaling near the band edges. The former became a long-standing puzzle, particularly in numerical calculations, when different types of boundary conditions have led to unambiguous results, doubting in the justification of finite-size scaling scenarios. The latter has been investigated by the transfer-matrix (TM) computations for the energies beyond the unperturbed band, however no clear critical behaviour was found and a reliable determination of ν failed. Moreover, the applicability of the scaling hypothesis far from the band centre has been questioned in recent studies [3].

Practically the critical parameters, like the critical exponent and the critical line of the phase diagram of the localization trajectory $f_c(E,W) = 0$ in the energy-disorder plane, can be explored by performing numerical-scaling simulations, since standard analytical approaches in many cases break down close to the transition. Under certain symmetry conditions it is natural to expect that the influence of boundaries on scaling properties become negligible, as the size of the system grows. Eventually in the thermodynamic limit the critical parameters should not depend on boundary conditions, as assumed by universality of the critical point. To the best of our knowledge, the invariance of the critical exponent ν with respect to change of the type of boundary conditions has not been examined yet.

Despite that the independence of the critical exponent on the distribution of the random potential has been verified, various numerical works concluded that ν changes by varying the position of the mobility edge, in contradiction to claims of the field theory. Therefore, investigating the detailed scaling behaviour along the phase localization trajectory is imperative since it gives insights into universal character of the Anderson transition.

Previous computational efforts using the transfer-matrix method have mostly been concentrated on the centre of the energy band $E = 0$, yielding the value $\nu = 1.5$ [3]. Here the scaling functions for various symmetry classes and the corresponding critical exponents have been determined with a high accuracy.

Boundary conditions

We choose two types of boundary conditions, periodic BC and Dirichlet BC, which belong to the same symmetry class (orthogonal), but are of essentially different topology. First we investigate the influence of different types of boundary conditions on the localization properties of the 3D disordered systems. The Green's function method combined with the transfer-matrix computations is used to obtain the localization length and the corresponding scaling function. In addition, the scaling behaviour is re-examined not only near the band centre of the Anderson model, but also near the band edges. The calculations of the localization length in quasi-1D geometry have been performed for the bar-shaped system of different cross-section ranging from L = 4 up to 14. We use the Anderson model with diagonal disorder:

$$H = \sum_{n\sigma} \varepsilon_r \left| r \right\rangle \left\langle r \right| + \sum_{r,\Delta} V_{r,r+\Delta} \left| r \right\rangle \left\langle r + \Delta \right|, \tag{1}$$

Here the electron states $|r\rangle$ are defined on the sites of a simple cubic lattice. The site energies ε_r are random entities, which are distributed uniformly in the interval from –W/2 to W/2. As for the tight-binding approximation, the coupling only between nearest neighbouring r and $r + \Lambda$ is taken into account. All energies are measured in units of the hopping matrix element V and lengths in units of the lattice constant $a = 1$.

Our numerical algorithm is based on the evaluating the Green's functions $G_M(L,W,E)$ of a one-particle with energy E, travelling in a bar-shaped disordered system of a length L and of a finite cross-section M^2, which connected to the two semi-infinite perfect leads. The localization length can be obtained in the quasi-1D limit of a long stripe or of a bar, L >> 1, using the Oseledec's theorem [2]. Then one has the following:

$$\frac{1}{\lambda_M(W,E)} = \lim_{L\to\infty} \frac{\ln |\, G_M(L,W,E)\,|}{L}, \tag{2}$$

Thus, the inverse localization length is simply the exponential decay rate of the spatial extension of $G_M(L,W,E)$. In practice, the study of the Green's functions is mapped into the equivalent transfer-matrix calculations. The latter yields the smallest positive Lyapunov exponent identified as λ_M^{-1}. Due to the convergence process of the underlying iteration procedure in the limit of large L, the statistical quantity λ_M becomes self-averaging. Thus the conventional averaging over a large ensemble of samples can be eliminated.

As a check, we have first examined the case of zero magnetic field $\alpha = 0$, extensively investigated previously. The reduced localization length Λ_M is computed as a function of the disorder strength W at a given energy $E = 0$, as shown in Fig.1. The curves for different sample sizes $M = 4$ - 18 all cross at a fixed point $W = W_c$, giving $\Lambda_M = 0.58$, which is independent of the size M within the statistical error bars. At $W < W_c$, the data for Λ_M continuously increases with increasing M, while at $W > W_c$ the sign of the size effect is opposite. This is a typical critical behaviour of the disorder induced metal-insulator transition. The critical value of disorder can be estimated as $W_c = 16.5$.

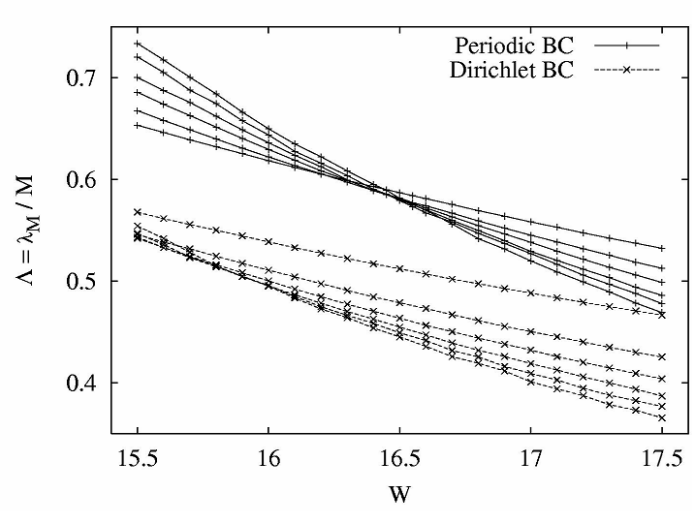

FIG.1 Renormalized localization length Λ as a function of disorder W for two different types of the boundary conditions. Data correspond to the energy $E = 0$ for various system sizes $L = 4,6,8,10,12$ and 14 (from smaller to larger steepness)

All the data for the reduced localization length Λ_M obtained by the TM-method have accuracy between 0.1% and 0.25% for the size M ranging from 4 up to 18. To get this accuracy around 3106 iterations are necessary. Further increase of the system size above M = 18 requires an improvement of the statistical accuracy of the raw data. Practically, the computation efforts (the CPU time) grow proportionally to M^7/ε^2, where $\varepsilon = \delta\Lambda_M / \Lambda_M$ is the relative statistical accuracy. The coefficient of proportionality depends on the type of the problem and on the efficiency of the computer and the optimization of the algorithm. For instance, on Unix 4.0F it is around 10^{-9} for the centre of the band $E = 0$ and the disorder $W = 16,5$, if the CPU-time is measured in seconds. Therefore the large-scale calculations are extremely time-consuming due to rather slow convergence process. Already for the size $M = 30$ and the error $\varepsilon = 0{:}5\%$ the one-processor CPU-time on Alpha-DEC computer (Unix 4.0F) exceeds several days.

Localization trajectory

We have calculated Λ for negative part of energies (near the left band edge). One can see that there is no common crossing point for the sizes considered. Therefore it is not feasible to detect critical behaviour, in spite of high accuracy. For even linear sizes $L = 2n$, where n is integer, the behaviour of Λ is symmetric with respect to the band centre $E = 0$, while for the odd sizes $L = 2n$-1 the energy dependence of Λ for negative energies differs from that for positive E.

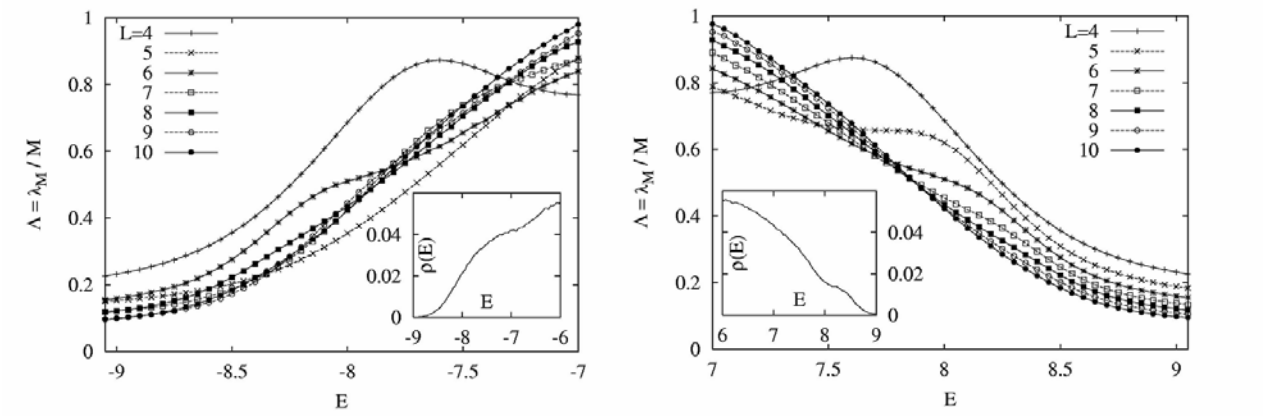

FIG. 2. Renormalized localization length Λ as a function of energy E near the left and right band edges for disorder strength W = 12. Insets show the density of states $\rho(E)$ for $L = 5$ at the same disorder W

However this difference diminishes with increasing the size of the system. One can expect that for considerably larger systems one could observe the common crossing point and locate the critical energy more precisely. The reason for this asymmetry is related to the asymmetry of the density of states for the odd *L*. In order to check this relation we have computed the exact energy levels corresponding to the Anderson Hamiltonian with periodic boundary conditions. The eigenvalues have been obtained by the direct diagonalization, by using the Lanczos algorithm. The insets in Fig.2 demonstrate the density of states for $L = 5$, which is different depending on the sign of the energy *E*. For the even L the density of states is symmetric around $E = 0$, as expected. The localization trajectory is shown in Fig. 4 both in the presence of the magnetic field and without magnetic field.

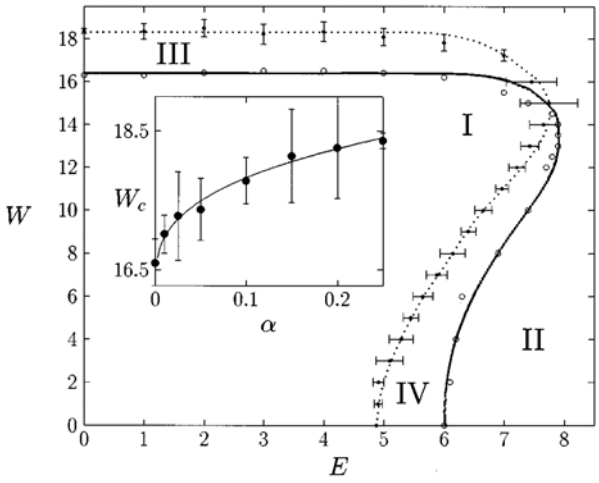

Fig. 4. The phase diagram of the Anderson model (localization trajectory). Open dots correspond to zero magnetic field. Full dots show the critical points $f(E_c,W_c)$ for a magnetic field $\alpha = 0{:}25$

Critical exponent

The question arises: what are the criteria to decide which way of analyzing the data is most reliable? The best criterion to my opinion is to be closer to the critical point and to operate carefully with the error bars. In general, from any statistical analysis of numerical data one could not say that the critical parameters equal with 100% (i.e. certainly) to some values, even though corresponding error bars are also determined. The problem of reliability of outcoming data should be always controlled by several independent methods.

The figure 5 demonstrates the disorder dependence of the localization length needed for the critical exponent ν and obtained from direct computer simulations for 3D disordered systems modelled by the Anderson Hamiltonian. It demonstrates a power law divergence of the localization length with the power equalling to critical exponent ν. This is one of the most distinguished achievements, since establishing the single-parameter scaling theory of localization by Abrahams and co-workers in 1979 [1]. It manifests itself a variety of calculation methods and disorder models used. Investigated are the problems with the time-reversal (no magnetic field or impurities) and the spin-rotational symmetry (no spin-orbit interaction). One can see from the fig. 5 that the most advanced and successful method is of the transfer matrices (TM).

An analytical approach based on the extension of 1D to higher dimensions has yielded the estimate ν =1,6, though relying on uncontrolled approximations. Recently, Kawabata has suggested a simple form for the β- function starting from the self-consistent considerations and derived a value $\nu = 1 + 1/\sqrt{3} = 1{,}58$, which strikingly well coincides with the latest findings by numerical modelling.

By combining the renormalization group treatment with the perturbative expansion to lowest order other researchers [4] have numerically extracted the value of the critical exponent $\nu_{RG} = 1{,}59$,

which was surprisingly close, for the first time, to the contemporary result, corresponding to our findings. Though being intensively investigated since the late fifties, the problem of the disorder-induced metal-insulator transition (MIT) of non-interacting electrons in three dimensions (3D) can be considered as being still unsolved.

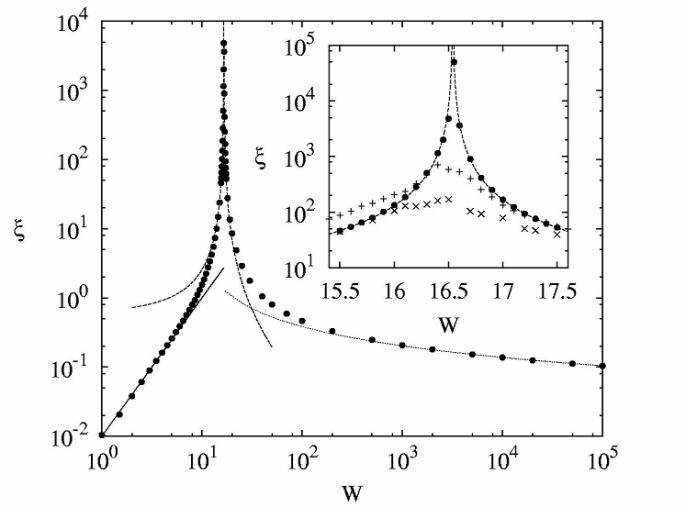

FIG. 5. The localization length ξ as a function of disorder W. Solid straight line is the weak-localization limit dotted line is the strong localization limit, and dashed line is the power-law, respectively. Inset: enlarged region in the very vicinity of $W = W_c$ (linear scale). Our results (•) are shown in comparison with those from Ref.[3, 4]

Conclusions

The influence of different types of boundary conditions on the Anderson transition is investigated by using the transfer matrix method. The finite-size scaling analysis is performed along the mobility edge trajectory, between the centre and the edge of the energy band. The critical exponent of the localization length proved to be independent of the type of boundary conditions, as well as of the energy, confirming the universality of the Anderson transition. By considering the lowest-order corrections to the single-parameter scaling, the critical exponent of the localization length is determined.

References

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ЛОКАЛИЗАЦИЯ ТРАЕКТОРИЯСЫ ЖӘНЕ СЫНДЫҚ ИНДЕКСІ

И.Х. Жәрекешев

Трансфер-матрицалар әдісімен хаостық жүйілердің электрондық локализациясы зерттелінеді. Локализация ұзындығының сындық индексі табылған.

ТРАЕКТОРИЯ ЛОКАЛИЗАЦИИ И КРИТИЧЕСКИЙ ИНДЕКС

И.Х. Жарекешев

Изучается электронная локализация хаотических систем методом трасфер-матриц. Найден критический индекс длины локализации.