Review of recent progress on numerical studies of the Anderson transition

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Abstract. A review of recent progress in numerical studies of the Anderson transition in three dimensional systems is presented. From high precision calculations the critical exponent $\nu$ for the divergence of the localization length is estimated to be $\nu = 1.57 \pm 0.02$ for the orthogonal universality class, which is clearly distinguished from $\nu = 1.43 \pm 0.03$ for the unitary universality class. The boundary condition dependences of some quantities at the Anderson transition are also discussed.

Keywords: finite size scaling, Anderson transition, universality

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1 Introduction

It is more than four decades since Anderson pointed out the existence of a disorder induced metal-insulator transition (the Anderson transition). After the discovery of the scaling behavior of conductance, it was realised that the transition is a second order phase transition. This naturally leads us to expect a degree of universality, i.e., the critical behavior does not depend on the details of the model but depends only on the basic symmetries of the system such as time reversal symmetry (TRS).

Numerical calculations have played a very important role in the investigation of random systems, for example percolating systems or spin glasses, where a quantitative understanding cannot be obtained with analytic methods. This is also true of the Anderson transition. In this paper, we review recent progress in numerical studies of the Anderson transition. Special emphasis is put on the universality of the exponent $\nu$ for the divergence of the typical length scales. We discuss the universal behavior of the statistics of energy levels and conductance at the transition. We finally comment on the boundary condition dependence of certain quantities such as level statistics, the conductance distribution function, and localization length.
2 Critical exponents

The Anderson transition is characterized by a vanishing conductivity, a diverging dielectric constant, and a divergence of the length scales as we change the parameter $x$ such as Fermi energy (electron density), impurity concentration, and pressure. Near the critical value $x_c$, the vanishing of conductivity $\sigma$ is described by the critical exponent $s$

$$\sigma \sim (x - x_c)^s,$$

(1)

and the divergence of the dielectric constant $\varepsilon$

$$\varepsilon \sim \frac{1}{(x_c - x)^s'}. \quad (2)$$

Here we suppose that $x > \langle x \rangle_c$ is the metallic (insulating) regime. In the metallic regime, the characteristic length scale $\xi$ is the correlation length, while in the insulating regime, it is the localization length. Both diverge with the same exponent $\nu$,

$$\xi \sim \frac{1}{|x - x_c|^\nu}. \quad (3)$$

From the scaling theory [2, 3, 4], the conductivity exponent $s$ and the length scale exponent $\nu$ are related

$$s = (d - 2)\nu \quad (4)$$

where $d$ is the dimensionality of the system. This is called Wegner’s scaling law. Numerical finite size scaling studies allow $\nu$ to be accurately determined, while in the experiments $s$ is measured.

The most accurate way of estimating the exponent $\nu$ is the transfer matrix method used in conjunction with finite size scaling [5, 6]. For three dimensional (3D) systems, we consider a very long bar with cross section $L \times L$. From the exponential decay length $\xi_L$ along the bar we define the dimensionless quantity

$$\Lambda_L = \frac{\xi_L}{L}, \quad (5)$$

and assume a single parameter scaling form,

$$\Lambda_L = f(\xi/L) = F(\delta x L^{1/\nu}). \quad (6)$$

where $\delta x = (x - x_c)/x_c$ is the distance from the critical point. Assuming that $\Lambda_L$ is an analytic function of $x$ for finite $L$, we expand $f$ as

$$\Lambda_L = \Lambda_c + a_1 L^{1/\nu}(x - x_c) + a_2 L^{1/\nu}(x - x_c)^2 + \cdots. \quad (7)$$

Fitting the numerical data to $f$, we estimate $\Lambda_c, \nu, x_c$ and the expansion coefficients $a_i$.

In some cases, such as quantum percolation where the lattice structure is disordered, the transfer matrix method is difficult to apply and we have to use other quantities which obey the single parameter scaling law $f$. The analysis of energy...
level statistics is free from the lattice structure problem. For example, when we diagonalize a $L \times L \times L$ cube and define $\Lambda_L$ by integrating the nearest neighbor level spacing $P(s)$ up to some point $s_0$

$$\Lambda_L = \int_{s_0}^{s_0} P(s) ds,$$

(8)

then the same scaling law is valid. In the insulating regime, in the limit of large $L$, $\Lambda_L$ approaches $\int_{s_0}^{s_0} P_{\text{Poisson}}(s) ds$ where $P_{\text{Poisson}}(s) = e^{-s}$ is the Poisson distribution. On the metallic side, it approaches $\int_{s_0}^{s_0} P_{\text{WD}}(s) ds$ where $P_{\text{WD}}(s)$ is the nearest neighbor spacing for Wigner-Dyson statistics. By making full use of scaling behavior, the exponent $\nu$ has been estimated for various models, and the universality of the transition confirmed with high precision.

2.1 3D Anderson model

The Anderson model has the Hamiltonian

$$H = \sum_{\langle i,j \rangle} V \exp(i\theta_{i,j}) C_i^\dagger C_j + \sum_i W_i C_i^\dagger C_i,$$

(9)

where $C_i^\dagger (C_i)$ denotes a creation operator of an electron at the site $i$ on the 3D cubic lattice and $W_i$ denote the random scalar potential at the site $i$. If the transition is universal, even when the distribution function of the random potential is changed, the critical exponent should be invariant. To demonstrate this, we set all the phases $\theta_{i,j}$ to be zero so that the time reversal symmetry exists (orthogonal universality class), and consider three different types of random potential: the box distribution

$$p(W_i) = \begin{cases} \frac{1}{W} & (|W_i| \leq W/2) \\ 0 & (\text{otherwise}) \end{cases},$$

the Gaussian distribution

$$p(W_i) = \frac{1}{\sqrt{2\pi}\sigma^2} \exp \left( -\frac{W_i^2}{2\sigma^2} \right),$$

with $\sigma^2 = W^2/12$, and the Lloyd model in which $W_i$ has a Lorentz distribution

$$p(W_i) = \frac{W}{\pi (W^2 + W_i^2)}.$$

For this distribution all moments higher than the mean are divergent and the parameter $W$ is proportional to the full width at half maximum of the distribution.

We then analyze the case when time reversal symmetry is broken by magnetic fields. If the transition is universal, the critical exponent should be independent of how we break the time reversal symmetry. We apply uniform magnetic fields and random magnetic fields. In the former case, the phases of the hopping are chosen so that the flux per unit square in the $xy$-plane is $1/3$ and $1/4$ of the flux quantum, while in the latter the phases of the hopping are random. In Table 1, we summarize the results of the critical exponents for various cases of the Anderson model. From this table, we see that $\nu = 1.57 \pm 0.02$ for the system with TRS. When the TRS is broken (unitary universality class) either by uniform or random magnetic fields, $\nu$ becomes $1.43 \pm 0.04$, clearly distinguished from that in the presence of TRS.
Table 1 The best fit estimates of the critical disorder $W_c$, $\Lambda_c$ and the critical exponent and their 95% confidence intervals. OB, OG, OL are for the system invariant under the operation of the time reversal with site potential distribution function box, Gaussian and Lorentz, respectively. In ref.[7], corrections to scaling are taken into account.

| Flux Type | $W_c$ | $\Lambda_c$ | $\nu$ | Ref. |
|-----------|-------|-------------|-------|------|
| OB        | 16.54(52,56) | 0.576(73,78) | 1.57(55,60) | |
| OG        | 21.29(27,32) | 0.576(73,78) | 1.58(55,61) | |
| OL        | 4.27(25,28)  | 0.579(76,88) | 1.58(46,65) | |
| Flux 1/3  | 18.316 ± .016 | 0.5683 ± .0013 | 1.43 ± .04 | |
| Flux 1/4  | 18.376 ± .017 | 0.5662 ± .0016 | 1.43 ± .06 | |
| Random flux | 18.80 ± .04  | 0.558 ± .003  | 1.45 ± .09 | |

2.2 Other models

If the Anderson transition is truely universal, the exponents should be the same, irrespective of whether we use the Anderson tight binding model or not. One example is the stack of quantum Hall layers, where electrons are allowed to hop from one layer to another [10, 11]. The critical exponent $\nu$ is estimated to be $1.45 \pm 0.15$, consistent with that in the case of Anderson model with broken time reversal symmetry.

Another important example is that of quantum percolation where the Hamiltonian is

$$H = \sum_{\langle ij \rangle} (t_{ij} C_i^\dagger C_j + h.c), \quad (10)$$

with the transfer integral

$$t_{ij} = \begin{cases} V \exp(i\theta_{ij}) & \text{ (for connected bond) } \\ 0 & \text{ (for disconnected bond) } \end{cases}, \quad (11)$$

Here we consider the bond percolation problem. Bonds are randomly connected with probabilities $p$. $\theta_{ij}$ is the Peierls phase due to magnetic fields. The underlying lattice is a three-dimensional cube of length $L$ with periodic boundary conditions imposed. As we increase $p$, we reach a geometrical percolation threshold $p_c$, and an infinite cluster is formed, however the wave functions are still localized and the system remains an insulator. If we further increase the probability $p$ and reach $p_q$, the wave functions become delocalized, and for $p > p_q$ current can flow through the system. This is the quantum percolation. Near the quantum percolation threshold $p_q$, the length scale diverges as $\xi \sim |p - p_q|^{-\nu}$.

As mentioned above, this model is difficult to study with the transfer matrix method, so the energy level statistics are used instead [12]. The estimate of $\nu$ is consistent with that of the Anderson model, $1.45 \pm .11$ with TRS ($\theta_{ij} = 0$), and $1.25 \pm .08$ in the absence of TRS where $\theta_{ij}$ is randomly distributed between $-\pi$ and $\pi$. The critical exponent indicates that quantum percolation may be in the same universality class as the Anderson transition [13].

$a$We usually use one standard deviation for error bar except in Table 1.
### 3 Scale invariance and boundary condition dependence at the transition

#### 3.1 Fractal dimension

We now turn our attention to the properties just at the Anderson transition. It is well known that at the transition, the wave function shows multifractal structure [14, 15, 16, 17, 18, 19, 20] which leads to the scale invariant behavior of conductance distributions [21, 22, 8, 23, 24, 25] and the energy level statistics [26, 27, 28, 29, 30, 31, 32, 33, 34].

The direct way to investigate the wave functions is to diagonalize the Hamiltonian. This, however, is strongly constrained by the limited memory and CPU time. Instead, we calculate here the time evolution of wave packets to extract the information of fractal dimension [35]. We first prepare the initial wave packet $|0\rangle$ close to the critical point by diagonalizing a small cluster located at the center of the system. The time evolution of the state at time $t$ is then obtained by

$$|t + \Delta t\rangle = U(\Delta t)|t\rangle$$

where $U(\Delta t)$ is the time evolution operator. We approximate $U(\Delta t)$ by a product of exponential operators

$$U(\Delta t) = e^{-iH\Delta t/\hbar} = U_2(p\Delta t)U_2((1 - 2p)\Delta t)U_2(p\Delta t) + O(\Delta t^3)$$

with $p = (2 - 2^{1/3})^{-1}$ and

$$U_2(\Delta t) \equiv e^{-iH_1\Delta t/2\hbar} \cdots e^{-iH_q\Delta t/2\hbar}e^{-iH_q\Delta t/\hbar}e^{-iH_{q-1}\Delta t/2\hbar} \cdots e^{-iH_1\Delta t/\hbar},$$

where $H_1, \cdots, H_q$ is a decomposition of the original Hamiltonian $H = \sum_i H_i$ in which each $H_i$ is simple enough to be diagonalized analytically [36, 37, 38, 39].

The square displacement of a wave packets is defined by

$$r^2(t) = \langle t|r^2|t\rangle.$$  

In metallic phase, $r^2(t)$ is proportional to $Dt$ where $D$ is the diffusion coefficient. In the insulating phase, it saturates to the square of localization length, $\xi^2$. At the critical point, the anomalous diffusion [40, 41]

$$r^2(t) \sim t^{2/d} = t^{2/3}$$

is expected.

The fractal dimension $D_2$ is estimated from the autocorrelation function

$$C(t) = \frac{1}{t} \int_0^t dt'|\langle t'|0\rangle|^2.$$  

Since $C(t)$ represents the inverse of the volume of the wave packet at time $t$,

$$C(t) \sim r^{-D_2},$$

from [41] we obtain

$$C(t) \sim t^{-D_2/d}.$$  

(17)
Fig. 1 $r^2(t)$ vs. $t$ at the critical point. Anomalous diffusion of $r^2 \sim t^{2/3}$ is observed.

Fig. 2 Autocorrelation function $C(t)$ as a function of time. Due to the fractal structure of the wave function, the decay of $C(t)$ is slow, $\sim t^{-0.43}$, compared to $t^{3/2}$ expected for normal diffusion.
Eq. (17) can be derived more rigorously in Fourier space \[20\].

In Figs. 1 and 2, we show the results of \( r^2(t) \) and \( C(t) \) at the transition in the presence of a uniform magnetic field. The strength of the field is \( 1/4 \) magnetic flux per unit square lattice in the \( xy \)-plane. The Anderson transition takes place at \( W_c = 18.4V \). By diagonalizing a small cluster of \( 7 \times 7 \times 7 \) located at the the center of the system, we follow the time evolution of wave packets in \( 101 \times 101 \times 101 \) systems. The geometric average of \( C(t) \) over 10 potential configurations are performed. By fitting the data for \( t > 40\bar{\hbar}/V \), the fractal dimensionality \( D_2 \) is estimated to be

\[ D_2 = 1.3 \pm 0.2 \]

considerably smaller than the space dimension \( d = 3 \). The above value is consistent with the estimate in the case of a random magnetic field \[9\] as well as lay ered systems in high perpendicular fields. \[42\]

3.2 Universal distribution functions and its boundary condition dependence

The above fractal structure at the transition leads to novel level spacing distribution \( P(s) \) and conductance distribution \( P(g) \) at the critical point. Recently, it was pointed out that \( P(s) \) and \( P(g) \) depend on the boundary condition \[43, 24\]. This was rather unexpected, since even completely different models show the same \( P(s) \) at the transition \[44\].

To investigate the origin of the boundary condition dependence, we study \( \Lambda_L \) with the fixed boundary condition (f.b.c.) imposed in the transverse direction of a long bar, and compare it with that in the case of periodic boundary condition (p.b.c.). For simplicity, we concentrate here on the Anderson model with orthogonal symmetry. In Fig. 3, we show the plot of \( \Lambda_L \) vs. the strength of randomness \( W \) for p.b.c. (+) and f.b.c. (○). The size \( L \) is 6,8,10 and 12, and the accuracy of raw data is 0.1%. The critical point should be indicated by a common crossing point in the data. We see that this is not clear for f.b.c. but seems to occur at \( W \approx 15.5V \), while data for p.b.c. indicate \( W \approx 16.5V \). This difference is physically unacceptable. In fact, a detailed study using \( \chi \)-square fitting makes clear that the simple single parameter scaling \[6\] fails.

To overcome this, we have to introduce corrections to scaling \[15, 7\] to take account of surface effects

\[ \Lambda_L = f(\delta wL^{1/\nu}, b(W)L^{-1}) \] (18)

with \( b(W) \) an analytic function of \( W \) around \( W_c \) and \( \delta W = (W - W_c)/W_c \). We then expand this expression as

\[ \Lambda_L = f_{\text{bulk}}(\delta wL^{1/\nu}) + f_1(\delta wL^{1/\nu})b(W)L^{-1} + f_2(\delta wL^{1/\nu})\frac{(b(W)L^{-1})^2}{2} + \cdots. \] (19)

Fitting the data to this expression neglecting higher order terms, we define the bulk part of \( \Lambda_L \)

\[ \Lambda_L^{\text{bulk}} = f_{\text{bulk}}(\delta wL^{1/\nu}) = \Lambda_L - f_1(\delta wL^{1/\nu})b(W)L^{-1} - f_2(\delta wL^{1/\nu})\frac{(b(W)L^{-1})^2}{2}. \] (20)
Fig. 3 $\Lambda_L$ vs. $W$ for p.b.c. (+) and f.b.c. (○). The size $L$ is 6,8,10 and 12.

Fig. 4 shows the results. Now a common crossing for f.b.c. is obtained at $W/V = 16.53 \pm .22$, and the critical exponent is estimated to be $1.61 \pm .16$, consistent with the p.b.c. case.

The above results indicate that even in the limit of infinite system size, $\Lambda_c^{\text{bulk}}$ depends on the boundary condition. $\Lambda_c^{\text{bulk}}$ is $0.576 \pm .001$ for p.b.c. and $0.419 \pm .03$ for f.b.c. This means that, when f.b.c. is adopted, the correlation length at the critical point for finite $L$ is significantly smaller, leading to the fact that $P(s)$ as well as $P(g)$ tends to share more features of an insulator. In fact $P(s)$ with f.b.c. is closer to a Poisson distribution, and the mean conductance $\langle g \rangle$ is smaller when f.b.c. is imposed.

4 Summary and concluding remarks

In this paper, we reviewed recent progress on the numerical study of the Anderson transition in three dimensional (3D) systems. Now the concept of the universality class is established numerically.

In spite of the fact that we can perform simulations for larger sizes in two dimensions, the estimate of the exponent is not as accurate as in 3D except for the quantum Hall case. For example, in the presence of spin-orbit scattering, the estimates of the exponent $\nu$ in 2D are rather scattered e.g. 2.2 [33], 2.5 [47] and 2.8 [15, 18], which can not be distinguished from the value of $\nu = 2.35 \pm .03$ obtained in the quantum Hall case. This may be due to the fact that the corrections to scaling is larger in 2D [47]. Further study is necessary to confirm the concept of universality in 2D systems.
Fig. 4 Same as Fig. but surface corrections are removed.

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