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Spectral Theory for Electronic States in One-Dimensional Disordered Systems*

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Spectral theory is employed to determine whether the states are localized or nonlocalized. The one-dimensional random Anderson model nearest-neighbor interaction is assumed. Eigenfunctions are numerically calculated and how the properties of eigenstates vary with the spread of random variables is examined. One striking feature is reported in the behavior of the degree of localization, which seems to support the Mott – C.F.O. conjecture.

A teoria espectral é empregada para determinar se os estados são localizados ou não. E usado o modelo uni-dimensional aleatório com interações entre vizinhos mais próximos, de Anderson. As auto-funções são calculadas numéricamente e examina-se como as propriedades dos auto-estados variam com a distribuição das variáveis aleatórias. Um ponto crucial é abordado no comportamento do grau de localização, o qual parece justificar as hipóteses de Mott – C.F.O..

1. Introduction

In recent years much attention has been paid to the research on amorphous materials. On the experimental side there are a number of properties that are characteristic of such disordered structures[1]. On the theoretical side, since the pioneer work of Anderson[2], a challenging problem to construct quantum mechanics of disordered systems still remains unsolved[3]. Real physical systems are obviously in three dimensions, but nevertheless the importance of one-dimensional systems cannot be ignored. Not only because it is quite desirable to understand such problems as the Mott-C.F.O. mode1[4] even in one-dimensional theories, but also because one is required to investigate

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organic materials which constitute the physical realization of the one-dimensional disorder[5].

During past years one of the main theoretical questions in disordered systems has been whether the eigenstates are extended or localized[6]. In one-dimensional systems it is known that all eigenstates are localized in the sense that the amplitudes of the states decrease exponentially at large distance. The result of analyses for higher dimensional systems is that all states are localized or the tails of localized states are separated from the band of extended states by a critical energy depending upon the degree of disorder. There is however some controversy about the exact value of this critica1 energy[7].

Quite naturally, the next questions are more detailed quantitative studies concerning the precise behavior of the density of states and the eigenstates. There have been many calculations[8-10] in the last few years and results obtained spread over a wide range of qualifications, which seem strongly dependent upon both the method and the model specifically employed. There may be, therefore, no need to explain much to justify any special motivation for our present research. However, it appears to us particularly that many research works thus far have leaned very much towards the analytical methods with formalistic mathematical arguments and are l e s practical in the sense that a group of states with exceedingly small level distance and binding energies are strictly distinguished as the localized states. On the other hand, numerical calculations on finite lattices are likely to prove useful for studying the properties of the localized states. Clearly any separation of the eigenstates of a finite system into a localized group and a non-localized group is rather optional.

The interesting question, and the one which concerns us here, is to determine how the spatial extent of the eigenstates varies with eigenvalues and with the degree of randomness of the system, and where non-localized states appear in the energy spectrum if they do. It seems exceedingly difficult to answer these quantitative questions by analytical methods, while a pure numerical study has its own defect in the sense that the results obtained largely depend upon the ways of calculation. It is sometimes not easy to distinguish systematic trends from the results. In this article, therefore, we take a somewhat intermediary method between those two. We use spectral theory instead of the usual self-energy calculation to determine whether the states are localized or nonlocalized. The one-dimensonal random Anderson model with

nearest-neighbor interaction is assumed. Eigenfunctions for this model are numerically calculated, and how the properties of eigenstates vary with the spread of random variables (site energies, possessing the Cauchy distribution) is examined. We discuss the results in the Section 3. Section 2 is devoted to present the spectral theory.

2. Spectral Theory

The idea of our computation is rooted in the method of spectral resolution. It is convenient to collect some well-known results about finite matrices which are fundamental for our subsequent analysis.

The Hamiltonian for the one-dimensional random Anderson model with nearest-neighbor interactions may be written as

$$H_{ij} = \varepsilon_i \, \delta_{ij} + V_{ij},$$

where the indices, i and j (=0,1, . . . , $n-1$), label the n sites of the lattice, ε_i is the energy associated with site i, and V_{ij} is the matrix element for hopping between sites, giving $-V$ for nearest neighbors and zero otherwise. The quantities ε_i are independent random variables possessing a distribution function $p(\varepsilon_i)$. To simplify numerical calculation, we use the Cauchy distribution; $p(\varepsilon_i) = (\gamma/\pi)/[\gamma^2 + \varepsilon_i^2]$. The Schroedinger equation $H\psi_\mu = E\psi_\mu$, ($\mu = 1,2, \ldots,$ n), is written as

$$VC_{i-1} + (\varepsilon_i - E)C_i + VC_{i+1} = 0, \tag{1}$$

$$\psi_\mu^+ = (C_0^{(\mu)}, \ldots, C_{n-1}^{(\mu)}),$$

where $C_{-1} = C_n = 0$, and we suppressed the superscript μ in Eq. (1) for simplicity. In order that these simultaneous equations may be solved, the determinant of the coefficients, designated by $P_n(E)$ should vanish. The equation $P_n(E) = 0$ determines eigenvalues $E_\mu^{(n)}$. Upon expanding $P_s(E)$ with respect to the last row or column, one finds

$$P_s(E) - (E - \varepsilon_{s-1}) P_{s-1}(E) + V^2 P_{s-2}(E) = 0, \tag{2}$$

which is valid for $s \geq 2$, if one defines $P_0(E) = 1$ and $P_1(E) = E - \varepsilon_0$.

The existence of the recurrence relation (2) enables us to establish a number of facts about the $E_\mu^{(n)}$ which will be needed later[11]. For example, the general behavior of these eingenvalues are investigated in terms of the following arguments: if $P_n(E)$ be a sequence of polynomials defined by equation (2), with $(-\varepsilon)$'s and V^2 positive quantities such

that $P_n(0) > 0$, the roots of $P_n(E) = 0$ are all distinct and negative, and separated by the roots of $P_{n-1}(E) = 0$. The inequality, $P_n(0) > 0$ can be examined and it it turns out that under the condition $(V^2/\varepsilon_i\varepsilon_{i-1}) \leqq 1/4$ for any i, it is satisfied even for the limit $n \longrightarrow \infty$ (Ref. 12).

To explain how to get the energy spectrum, let us first consider the simplest example where the random variables $\varepsilon_i = W$ are constant. The recurrence relations are then satisfied by the Chebyshev polynomials,

$$P_n(E) = v'' \sin\{(n+1)\omega\}/\sin o$$

where $\cos o = (E - W)/2V$. The zero points of $P_n(E)$ are obtained as $\omega_\mu^{(n)} = \mu\pi/(n+1)$; $\mu = 1, 2, \ldots,$ n. Eigenfunctions corresponding to eigenvalues $E_\mu^{(n)} = W + 2V\cos\{\mu\pi/(n+1)\}$ are denoted by

$$\psi_\mu^+ = \{\theta_\mu^{(n)}\}^{-1/2}\,(P_0(E_\mu^{(n)}),\ P_1(E_\mu^{(n)})/V, \ldots, P_{n-1}(E_\mu^{(n)})/V^{n-1}) \tag{3}$$

Here the normalization factor is evaluated as

$$\theta_\mu^{(n)} = [(n+1)/2]\sin^2\{\omega_\mu^{(n)}\}. \tag{4}$$

We define a spectral function $\rho^{(n)}(E)$ as follows: $\rho^{(n)}(E)$ is to be a non-decreasing step-function defined for $-\infty < E < \infty$, with discontinuity $1/\theta_\mu^{(n)}$ at $E = E_\mu^{(n)}$, $(\mu = 1,2, \ldots,$ n). Explicitly, it is written as

$$\rho^{(n)}(E) = \begin{cases} 0, & E \geqq E_1^{(n)} \\ \cdots & \\ \cdots & \\ -\left(\dfrac{1}{\theta_1^{(n)}} + \dfrac{1}{\theta_2^{(n)}} + \ldots + \dfrac{1}{\theta_r^{(n)}}\right), & E_{r+1}^{(n)} \leqq E < E_r^{(n)} \\ \cdots & \\ -\left(\dfrac{1}{\theta_1^{(n)}} + \dfrac{1}{\theta_2^{(n)}} + \ldots + \dfrac{1}{\theta_n^{(n)}}\right), & E < E_n^{(n)}. \end{cases}$$

Upon writing $\Delta\omega = \pi/(n+1)$, we find that

$$\{\theta_\mu^{(n)}\}^{-1} = (2/n)\sin^2\{\omega_\mu^{(n)}\}\,.\,A\ o$$

and by a formal limiting process $n \longrightarrow \infty$, we get

$$d\rho(E) = \frac{dE}{\pi V}\left[1 - \left(\frac{E-W}{2V}\right)^2\right]^{1/2}$$

The spectrum is hence continuous over the interval $W-2V \leqq E \leqq W+2V$ and the density of states is given by $d\rho(E)/dE$. It is also observed that as n goes to infinity, if any $\theta_\mu^{(n)}$ remains finite, there is a discontinuity at that point in the energy spectrum. This gives us a criterion for distinguishing localized and nonlocalized states.

We now return to the disordered case by allowing ε_i to be independent random variables commonly possessing the Cauchy distribution at each site. If we define $Z_s(\xi) = P_s(\xi)/VP_{s-1}(\xi)$, the recurrence formula (2) leads to

$$\{Z_{s-1}(\xi)\}^{-1} = (\xi - \varepsilon_{s-1})V^{-1} - Z_s(\xi) \,. \tag{5}$$

Since $Z_n(E_\mu^{(n)}) = 0$ we can successively get all Z's and therefore P's. To have orderly indices, let us introduce

$$t_0 = Z_n(E_\mu^{(n)}),\ t_1 = Z_{n-1}(E_\mu^{(n)}),\ \ldots,\ t_{n-1} = Z_1(E_\mu^{(n)})$$

and relabel $\varepsilon_{n-1}, \varepsilon_{n-2}, \ldots, \varepsilon_0$ as $E_1, \ldots, \varepsilon_{n-1}$. As it is easily recognized in the course of calculation, quantities with the dimension of energy appear only through the ratio with V (such as $\varepsilon_i/V, \gamma/V, \alpha/V, \lambda/V$ etc.) and hence the choice of V can be regarded as one of energy scale. This choice may therefore be made for computational convenience and hereafter we consider those quantities as measured in units of V.

We first treat a case $E_1 = 0$, the center of the band; here we fix the origin of energy in the distribution function $p(\varepsilon)$. Since the E_i are random variables, the quantities t_i become random variables with distributions $f_s(t_s)$ determined by[8]

$$f_s(t_s) = t_s^{-2} \int_{-\infty}^{\infty} p(t_{s-1} + t_s^{-1})\, f_{s-1}(t_{s-1})\, dt_{s-1}, \tag{6}$$

where $f(t_0) = \delta(t_0)$ and $p(\varepsilon) = (\gamma/\pi)/[\gamma^2 + \varepsilon^2]$. For this distribution of $p(\varepsilon)$, contour integration shows that

$$f_s(t_s) = (\alpha_s/\pi) / [\alpha_s^2 + t_s^2], \tag{7}$$

while $a_s = 1/(\alpha_{s-1} + \gamma)$ for $s \geqq 1$ and $\alpha_0 = 0$. As s goes to infinity, a_s tends to a limit a given by a positive root of $\alpha(\alpha + \gamma) = 1$, which is smaller than unity. One disadvantage of the Cauchy distribution is that with it the average value is zero and the root-mean-square deviation does not exist. It is therefore usual to calculate its average through the average of $\log t_s$ as $\bar{t}_s = \exp.\ \{\overline{\log t_s}\}$, and

$$2 \int_0^{\infty} f_s(t_s) \log t_s \, dt_s = \log \alpha_s.$$

The recurrence relation of Chebyshev polynomials $U_s(x)$ enables us to establish a simple result for a,;

$$\alpha_s = iU_{s-1}(i\gamma/2)/U_s(i\gamma/2),$$

where $U_s(x) = \sin[(s+1)\theta]/\sin 0$ and $x = \cos O$ It follows from definition of $Z_s(\xi)$ that

$$\overline{P_s(0)} = i^s\, U_{n-s-1}(i\gamma/2)/U_{n-1}(i\gamma/2).$$

As n increases towards infinity, the normalization factor tends to a limit, $\theta(0) \text{ r } \lim \theta^{(n)}(0) = a^2/(a^2-1)$ and since $a = (\gamma/2) + [1+(\gamma/2)^2]^{1/2}$, it it is finite unless $\gamma = 0$ (Ref. 13).

When the consideration moves away from the center of the band, i.e. $E_\mu^{(n)} \equiv \xi\, 1\, 0$, the equation (6) should be modified as

$$f_s(t_s) = t_s^{-2} \int_{-\infty}^{\infty} p(t_{s-1} + t_s^{-1} - \xi)\; f_{s-1}(t_{s-1})\; dt_{s-1}.$$

Again, for the Cauchy distribution $p(\varepsilon)$, we obtain
$f_s(t_s) = (\alpha_s/\pi)/[\alpha_s^2 + (t_s - \lambda_s)^2]$, where

$$\alpha_s = \frac{\alpha_{s-1}+\gamma}{(\alpha_{s-1}+\gamma)^2 + (\xi-\lambda_{s-1})^2},\quad \lambda_s = \frac{\xi-\lambda_{s-1}}{(\alpha_{s-1}+\gamma)^2 + (\xi-\lambda_{s-1})^2},$$

and $\alpha_0 = \lambda_0 = 0$.

3. Results of Numerical Computation

It is natural to inquire a little more closely into the nature of the spectral function which has appeared in the preceding section. We recall that the roots of $P_n(\xi) = 0$ ($n \geqq 1$) are distinct and negative and are separated by the roots of $P_{n-1}(\xi) = 0$, provided that $P_n(0) > O$ (Remind that we shift the origin of energy later upon introducing the distribution $p(\varepsilon)$.) It then follows from our definition of $E_r^{(n)}$ that for fixed $r \geqq 1$, $E_r^{(n)} > E_{r+1}^{(n)}$. If we assume that $E_r^{(n)}$ tends to a limit as n goes to infinity, say $E_r^{(n)} \longrightarrow E_{,,}$ it is clear that $E_1 > E_2 > \ldots$. Then $\rho(E)$ is a step function with discontinuity $1/\theta_r$ at $E_{,,}$ where $1/\theta_r = \lim_{n\to\infty} 1/01'$. Of course, unless any restrictions are put on ε_i, nothing can be said about the energy spectrum, and they cannot be easily related to the function

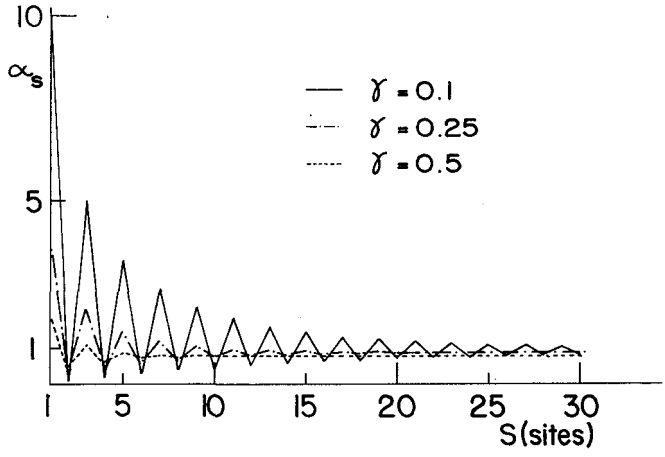
10
α_s
5
1
γ = 0.1
γ = 0.25
γ = 0.5
1
5
10
15
20
25
30
S(sites)

Fig. 1a

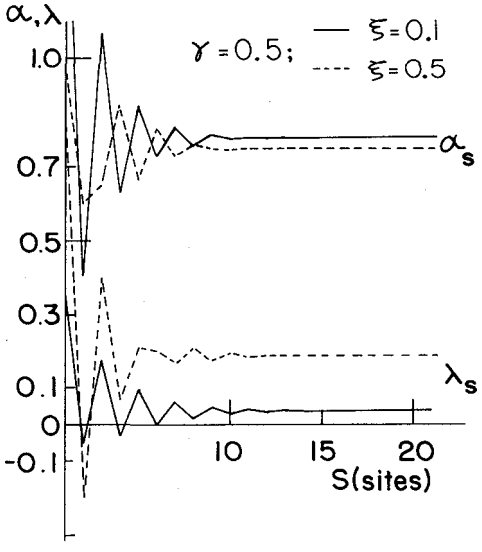
α, λ
1.0
0.7
0.5
0.3
0.1
0
-0.1
γ = 0.5;
ξ = 0.1
ξ = 0.5
α_s
λ_s
10
15
20
S(sites)

Fig. 1b

$\rho(E)$. However, it may happen that 8, is infinite and the discontinuity at E, is zero. This is our present concern for the Cauchy distribution of ε_i. The advantage of the present analysis is that we are always able to deal with the infinite lattice, even though we need not calculate. As is well known, to obtain results by analytical methods it is necessary to make some very restrictive arguments using the limit n $\longrightarrow \infty$ whose validity is extremely difficult to prove mathematically rigorously. It is therefore important that numerical results be available even if only for simple models.

We may be allowed to regard γ and $1/\theta_r$ as parameters designating degree of randomness and degree of localization, respectively. Fig. la and lb demonstrate rather rapid convergence of a, and λ_s in Eq. (8) with respect to the site number. This is true for relatively large y, but as γ becomes smaller, the rate of convergence decreases very sharply. For example, 60 sites are required to converge for $\gamma = 0.1$ and at least 120 sites are necessary for $\gamma = 0.05$ before approximate convergence. It is illustrated in Fig. 2 that the average wavefunctions decrease quickly with the distances as the degree of randomness increases, but their tails become longer and longer as γ becomes exceedingly small. It is thus confirmed that for a far smaller degree of randomness (y = 0.01 or less) the wavefunctions spread progressively over a huge number of sites. This extremely long tail is due to the Cauchy distribution.

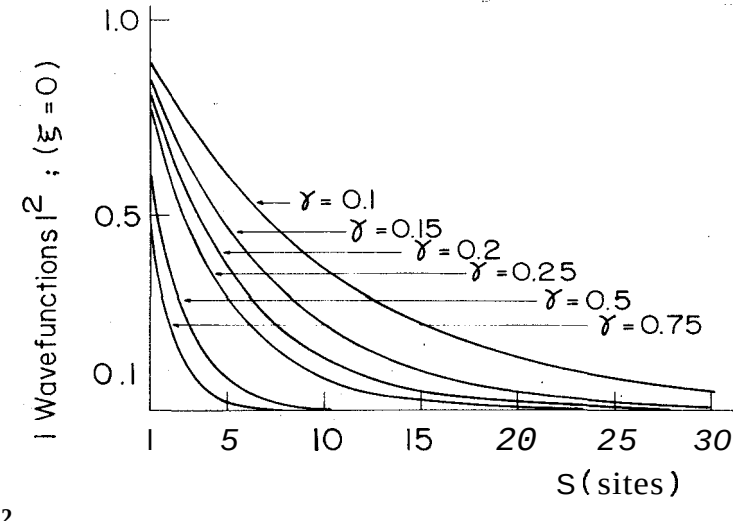

Fig. 2

We calculate $1/\theta(0)$ for these wavefunctions. Fig. 3 shows that the discontinuity at $\xi = 0$ (the center of the band of $p(\varepsilon)$) becomes bigger and bigger as y increases.

Our snalysis is related to the previous work[8] in which its authors examined convergence of the self-energy in the perturbation series. The uniform convergence of the distribution $f_n(x)$ to $f(x)$ as $n \longrightarrow \infty$ is reduced to that of two continued fractions (8) since the Cauchy distribution forms a closed system under the convolution. For $5 = 0$, all A, are zero and a, tends to a limit a as $s \longrightarrow \infty$. As was already shown, the limit $\theta(0)$ is finite unless $\gamma = 0$.

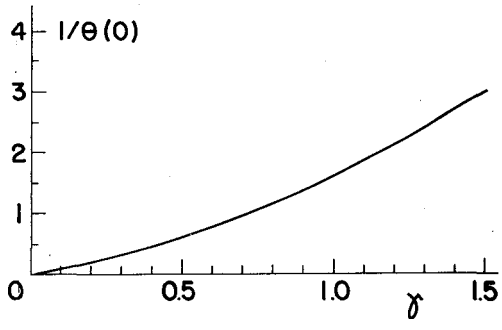

Fig. 3

The next step is to find any systematic trends of $\theta(\xi)$ with ξ. The convergence of the continued fractions (8) is numerically confirmed up to $y = 0.05$. For fixed y, the speed of convergence in a, and λ_s increases with the magnitude ξ. To calculate $\theta(\xi)$, however, we have to surmount the difficulty (of the Cauchy distribution) in defining its average value. It is easy to find that the average $\bar{t}_s$ lies between $|a, -\lambda_s|$ and $|a, +A, |$. We also take into account the intermediate value $(\alpha_s^2 + \lambda_s^2)^{1/2}$ and draw figures of $1/\theta(\xi)$ for these three values $(|a, -A, |, (\alpha_s^2 + \lambda_s^2)^{1/2}, |\alpha_s + \lambda_s|)$ classifying A, B and *C*, respectively. It is shown in Fig. 4 (case **A**) that states become more localized as the eigenvalue increases. Since the minimum value is assumed for the wavefunction, the rate of increase is very sharp, while we see in Fig. 5 for case B that the curves keep constant up to a given energy and then increase outside this value. It is clear that the degree of randomness augments localization of states. A striking feature, however, appears in the curves for case C. The function $1/\theta(\xi)$ decreases once and then rises again somewhere around $\xi = 1.1$. Fig. 6 illustrates that the discontinuity becomes very small for those values of y below 0.5, and the region of vanishingly

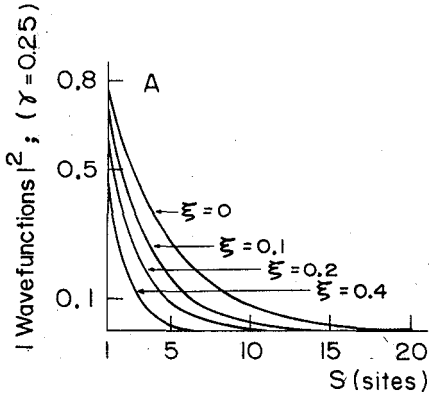

Fig. 4a

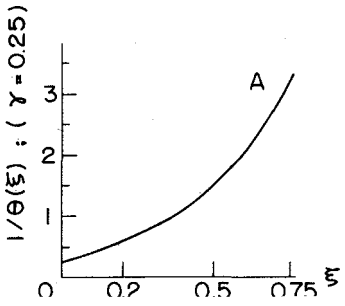

Fig. 4b

small values of $1/\theta(\xi)$ increases with decrease of y. As we assume the maximum value for the wavefunctions, this does not seem to occur with appreciable probability in the infinite system. Actually, for almost all members of the ensemble the results of case B or the ones close to them should be applied. As a general trend, however, our result clarifies how and where the localization of states increases with the degree of randomness. The result indicating the increase of localization at the center of band is hard to explain, but similar situations have been reported in numerical studies of another model. Its interpretation is attempted there by the author[g] in terms of the effects of the lattice size. In our analysis we have one end point even after we take the limit $n \longrightarrow \infty$. This may cause some effects.

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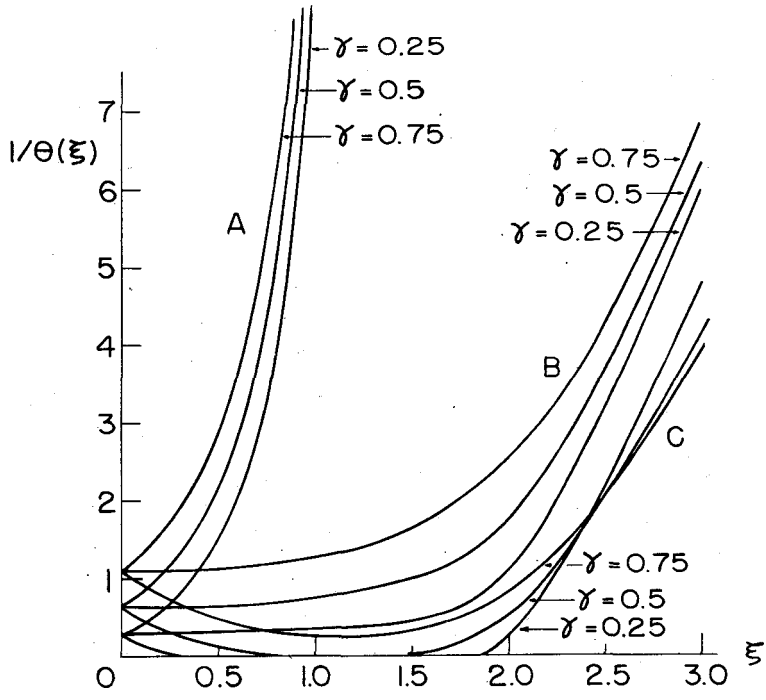
γ = 0.25
γ = 0.5
γ = 0.75
1/θ(ξ)
A
γ = 0.75
γ = 0.5
γ = 0.25
B
C
γ = 0.75
γ = 0.5
γ = 0.25
ξ
0
0.5
1.0
1.5
2.0
2.5
3.0
1
2
3
4
5
6
7

Fig. 5

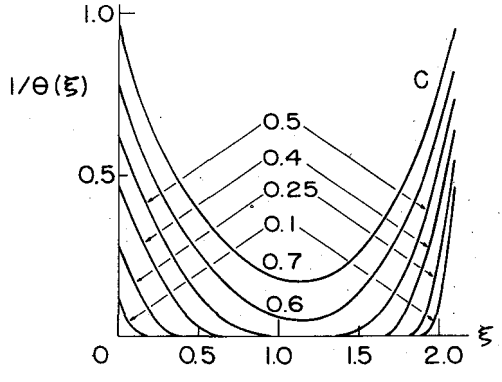
1.0
1/θ(ξ)
0.5
C
0.5
0.4
0.25
0.1
0.7
0.6
ξ
0
0.5
1.0
1.5
2.0

Fig. 6

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