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Stability of Localized States and Sum of Random Variables

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An iterative solution of the integral equation in a self-consistent theory of localization is investigated for onedimensional disordered systems. The solution is a distribution function for a sum of random variables. Therefore, the central limit theorem in probability theory is related with it and a new idea is introduced on the problem of localization.

Foi investigada uma solução iterada para a equação integral da teoria auto consistente de localização em sistemas desordenados unidimensionais. A solução é uma função distribuição para soma de variáveis aleatórias. Uma nova idéia no problema de localização e introduzida relacionando-se a solução com o teorema do limite central.

1. Introduction

A statistical approach to the problem of localization in disordered systems was developed by Abou-Chacra et *al.* (1973) (referred to as I). in which a self-consistent condition with the form of an integral equation is imposed on a probability distribution for the values of the self-energy. A scheme of practical calculation is simple in one dimension where the integral equation is linear. However, a solution by Beeby (1973) (referred to as II) to the problem is an approximate solution valid only for large values of an independent variable. In this paper we will search for an exact solution of the integral equation. It is shown thar the solution is related to the central limit theorem in probability theory about a sum of random variables. This discussion is contained in § 2. The effect of the real part of the self-energy on the imaginary part is accurately analyzed in § 3.

2. The Integral Equation and its Solution

Let us consider a system in which an electron moves between sites i on which it has energy levels ε_i. The quantity ε_i is regarded as a random

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variable with a certain distribution. Though not necessary, it is simplest to assume that the matrix-element for hopping between sites is $-V$ for nearest-neighbour interaction but zero otherwise. For the self--energy $S_i(E) = E_i - i\Delta_i$, where $E = R + i\eta$, we have

$$E_i = \sum_j |V_{ij}|^2/(R-\varepsilon_j-E_j),$$

$$\Delta_i = \sum_j |V_{ij}|^2 \ (\eta+\Delta_j)/(R-\varepsilon_j-E_j)^2. \quad (1)$$

The eigenvalue unity of the latter's homogeneous equation corresponds to the limit of stability of the localized states [I, Eq. (4.7)].

In one dimension this equation, for the imaginary part of the self--energy, is written as

$$y_{j+1} = \log(V/R-\varepsilon_j)^2 + y_j, \quad (2)$$

where $\Delta_i(E) = \eta\, d_i(E)$ and $y_i \equiv \log d_i(E)$, [11, Eq. (6)][4]. In deriving Eq. 2, the equation is simplified by ignoring for the moment the real part E_j of the self-energy. Localized states are characterized by the imaginary part $\Delta_i(E)$ tending to zero with probability unity as η goes to zero. The self-consistent probability of y is determined by an integral equation

$$f(y) = \int^{c} p(x) f(y-x)\, dx, \quad (3)$$

where the quantity $p(x)$ is a distribution function of the random variable $x = \log(V/R-\varepsilon)^2$. For site energies uniformly distributed between $-W/2$ and $W/2$, and $R = 0$, we have

$$p(t) \equiv p(x)\ (dx/dt) = \theta(t)\ \exp(-t), \quad (4)$$

with definitions, $t = (x-b)/2$ and $b = 2\log(2V/W)$. With respect to this distribution, the mean value $\bar{x}$ and the root-mean-square deviation are $b+2$ and 2, respectively.

The function system $\gamma(t, s) = t^{s-1} \exp[(-t)/\gamma(s)]$, called the Γ-distribution, forms a closed system under the convolution. Hence, when we solve Eq. (3) by iteration with an initial function $f_0(t) = \delta(t)$, we find $f_n(t) = \gamma(t, n)\,\theta(t)$. If we introduce $z = t - 1$ (so tha $\bar{z} = 0$), we can write

$$f_n(z) = e^{-(z+n)}(z+n)^{n-1}\ \theta(z+n)/\Gamma(n), \quad (5)$$

and it follows that $f_n(z)$ approaches a constant as n increases indefinitely. Thc Γ-distribution does not satisfy the Lindeberg condition (which is necessary and sufficient to the central limit theorem) and the function $f_n(z)$ does not, therefore, approach the Gaussian distribution.

On the other hand, if we take the Cauchy distribution, $(\gamma/\pi)/\gamma^2+\varepsilon^2$, the function f_n approaches the Gaussian distribution. Introducing $b'=\log\,(\gamma/V)^2$, $x=\log\,(\gamma/\varepsilon)^2$ and $t=(x+b')/\pi$, we get

$$p(t)=\Gamma\left(\frac{1}{2}+\frac{i}{2}\,t\right)\Gamma\left(\frac{1}{2}-\frac{i}{2}\,t\right)\Big/2\pi. \tag{6}$$

The average value $\bar{x}$ and the root-mean-square for this distribution are $-b'$ and π, respectively. Upon solving Eq. (3), for p of Eq. 6, iteratively, starting with the delta function, we are led to

$$f_n(t)=[2^{n-2}/\pi\Gamma(n)]\left|\Gamma\left(\frac{n}{2}+\frac{i}{2}\,t\right)\right|^2, \tag{7}$$

and

$$\lim_{n\to\infty} f_n(t)=\lim_{n\to\infty}\,(2\pi n)^{-1/2}\,\exp\,(-t^2/2n). \tag{8}$$

Since the self-consistent probability in II is only an approximate solution, we cannot derive Eq. (7) of that article. We are, however, able to find the limit of stability of the localized states by a different discussion. Let us consider to solve Eq. (2) by iteration and set R = 0 for simplicity. The sum y of random variables has the mean values $\lim n(b+2)$ for the distribution (4). To avoid growing up of $\bar{y}$ indefinitely with n, it is necessary that the average $\bar{x}=b+2$ should be zero. However, as $-\infty$ for logd only results in $d=0$, the value $b+2$ has only to be less than zero; $b\leq-2$, or the critical value $V_c=W/2e$. By the same argument, one finds the critical value V_c for the distribution (6); $b'\geq 0$ or the critical value $V_c=y$. Moreover, it is observed from (Eq. 5) and (Eq. 8) that the distribution function spreads more and more as n increases and finally spreads over the infinite range, manifesting breakdown of the stability of the localized states.

3. The Effect of the Real Part

We will next investigate the effect of the real part of the self-energy, tentatively ignored in the previous section. The result shows tbat its effect is crucial. The simplest case to study is the Cauchydistribution of site energies, since in that case the self-consistent equation for the real part is exactly solved.

Introducing a variable $t_j = E_j/V$, we have for the real part of the self energy,

$$t_{j+1}^{-1} = (\mathrm{R} - \varepsilon_j)/V - t_j$$

and, for its distribution at $\mathrm{R} = 0$,

$$f(t) = t^{-2} \int_{-\infty}^{\infty} p(t' + t^{-1})\, f(t')dt', \tag{9}$$

where $p(t) = (\gamma'/\pi)/\gamma'^2 + t^2$ and $\gamma' = \gamma/V$. A solution of this integral equation is given by $f(t) = (\alpha/\pi)/\alpha^2 + t^2$ and the parameter is a continued fraction defined by $\alpha(\alpha + \gamma') = 1$. Let us consider now a sum of two random variables, ε_j and E_j, when both have the Cauchy distribution but different values of width-parameters. It is easy to prove that a distribution for the sum is also the Cauchy distribution with a width given by a sum of each width. Therefore, the inclusion of the effect of E_j in Eq. (1) is achieved by replacing the parameter γ' by $a' = \gamma' + a$ in the distribution of ε_j. Accordingly, one obtains

$$a' = (\gamma'/2) + [1 + (\gamma'/2)^2]^{1/2} \geq 1.$$

In Eqs. (8) and (5), we have employed variables whose average values and the root-mean-square deviations are zero and unity, respectively. Going back to the original variable y, we have for Eq. 8

$$\lim_{n\to\infty} f_n(y) = \lim_{n\to\mathrm{m}} \exp\ [-(y+nb')^2/2n\pi^2]/(2\pi^3 n)^{1/2},$$

which vanishes for positive y if $b' > 0$ no matter how small it is. We have $b' = \log a' > 0$ unless $\gamma' = 0$. Since the imaginary part of the self-energy is $\eta \exp(y)$, there is no possibility that y becomes infinitely large so that the imaginary part may be finite as η goes to zero.

In conclusion, to solve iteratively the self-consistent integral equation for the imaginary part of the self-energy in one dimension leads to finding a distribution function for a sum of random variables. From each site of lattice points there is a small contribution (to the imaginary part of the self-energy)as a random variable with a certain distribution. Their sum becomes larger as the site number increases and the distribution of the sum approaches the Gaussian distribution under the Lindeberg condition. Moreover, the distribution function finally spreads over the infinite range and shows breakdown of the stability of the localized states. The finiteness in the mean value of the sum gives the criterion for the onset of localization, which is different in appearance from those given by Ziman[3]. The effect of the real part of the self-energy on the imaginary part is also analyzed for the Cauchy distribution of site energies. Its role is essential to obtain the known result about the localized states in one-dimensional disordered systems. Throughout this paper we have set $R = 0$, but it is possible to remove this condition. It seems interesting to consider the extension of the present consideration into higher dimensions by studying the self--consistent non-linear integral equation.

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4. In deriving this equation, the approximation is done that the d, are larger than unity.