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Anomaly in the Band Centre of the One-Dimensional Anderson Model*

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We calculate the density of states and various characteristic lengths of the one-dimensional Anderson model in the limit of weak disorder. All these quantities show anomalous fluctuations near the band centre. This has already been observed for the density of states in a different model by Gorkov and Dorokhov, and is in close agreement with a Monte-Carlo calculation for the localization length by Czycholl, Kramer and MacKinnon.

1. Introduction and Results

Recently, Czycholl, Kramer and MacKinnon [1] have calculated the localization length and the conductivity in a one-dimensional Anderson model (nearest neighbour off-diagonal elements $-V$, width W of the rectangular distribution of the diagonal matrix elements) using a new numerical technique. They found that the localization length given by the increase of the average logarithmic amplitude for an eigenfunction with fixed boundary condition at one end and given energy E

$$\xi_0^{-1} = \lim_{r\to\infty} \frac{1}{r} \langle \ln(|\psi_{r+1}|^2 + |\psi_r|^2)^{1/2} \rangle \tag{1}$$

($\langle \ldots \rangle$ indicates the ensemble average) obeys

$$\xi_0 = (104 \pm 1)\, V^2/W^2 \tag{2}$$

in the centre of the band for weak disorder. Thouless [2] finds from a perturbation theory to second order in the diagonal matrix elements

$$\xi_0 = (96V^2 - 24E^2)/W^2 \tag{3}$$

Here we show that there is an anomaly in the centre of the band which yields for $E \ll V$ and $W \ll V$

$$\xi_0 = V^2 W^{-2} f(6EV/W^2) \tag{4}$$

with $f(0) = 105.045$ in close agreement with Czycholl, Kramer and MacKinnon and $f(\pm\infty) = 96$ in agreement with Thouless. An indication that the perturbation expansion by Thouless breaks down at zero energy is obtained from the fourth order term which diverges at this special energy (it is the contribution $\sum_{jk} G^0_{ij} G^0_{jk} G^0_{kj} G^0_{jk} G^0_{ki}$ in (6.13) of [2]).

A similar anomaly for the density of states ρ has already been observed by Gorkov and Dorokhov [3]. Due to a "dispersion" relation by Thouless [4] which connects ρ and ξ_0 one has to expect an anomaly for ξ_0, too. This anomaly is a resonance effect. It occurs at the energy which obeys $E^0(q) = E^0(3q)$ where $E^0(q)$ is the energy dependence on the wavevector q for vanishing disorder. (This can be obtained from the fourth order term mentioned above).

Besides ξ_0 and ρ we consider two other lengths $\hat{\xi}$ and ξ_1 which describe the decay of the eigenstates and the phase fluctuations in the eigenfunction $\psi(r)$ at large distances

$$\langle |\psi(r)\, \psi(r)| \rangle \sim \exp(-|r-r'|/\hat{\xi}) \tag{5}$$

$$\langle \psi(r)\, \psi(r') \rangle \sim \exp(-|r-r'|/\xi_1) \cos(\kappa |r-r'|) \tag{6}$$

for which we observe similar anomalies. The results are summarized in Table 1. For the Anderson model

$$\hat{\eta} = W^2/12V^2, \quad x = 6EV/W^2 \tag{7}$$

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Table 1. Numerical values of the lengths ξ and the density of states ρ in the limit $E \ll V$, $W \ll V$. All quantities are explained in Sect. 1

	$E=0$ exact	$E=0$ approximation (87)	asymptotic $(x \gg 1)$
$\hat{\xi}\hat{\eta}$	17.71622	17.655	$16+27/(32x^2)+\ldots$
$\xi_1\hat{\eta}$	4.24332	4.235	$4+9/(32x^2)+\ldots$
$\xi_0\hat{\eta}$	8.75376	8.727	$8+3/(8x^2)+\ldots$
$2\pi V\rho$	1.01508	1.014	$1-1/(128x^2)+\ldots$

the results hold for a more general distribution of the diagonal-matrix elements ε. If the ensemble averages of ε vanish and if the variance of ε is finite, then

$$\hat{\eta}=\langle\varepsilon^2\rangle/V^2, \quad x=EV/2\langle\varepsilon^2\rangle \tag{8}$$

In Sect. 2 we describe the model. Basically we follow the technique first introduced by Schmidt [5], further developped by Halperin [6], Gorkov and Dorokhov [3], Wegner [7] and Kunz and Souillard [8]. In [3] only the density of states is considered. References [3, 6, 7] were applied to models which are not directly related to the Anderson model. Although [8] can directly be applied to the Anderson model, it is convenient in the limit of weak disorder to introduce phase variables instead of the ratios of amplitudes used by Kunz and Souillard. The corresponding equations for ρ and the ξ's are developped in Sects. 3 and 4. The limit of weak disorder is considered in Sect. 5. Basically ρ and the ξ's are determined from the eigenvalues and eigenfunctions of integral kernels. The eigenvalues of these kernels become highly degenerate for vanishing disorder at zero energy. Thus, a single perturbation theory which yields (2) breaks down and degenerate perturbation theory which yields (4) has to be used.

2. Model

We consider the one-particle Hamiltonian

$$H=-V\sum_{l=1}^{N-1}(c_l^+ c_{l+1}+c_{l+1}^+ c_l)+\sum_{l=1}^{N}\varepsilon_l c_l^+ c_l \tag{9}$$

where c_l^+ and c_l are the creation and annihilation operators of the electrons at sites $l=1,2\ldots N$. V is a positive constant, the ε's are independent random variables distributed according to

$$dP_N=\prod_{l=1}^{N}(p(\varepsilon_l)\,d\varepsilon_l) \tag{10}$$

The eigenstates of H

$$|\psi\rangle=\sum_l \psi_l|l\rangle \tag{11}$$

obey

$$-V\psi_{l-1}+\varepsilon_l\psi_l-V\psi_{l+1}=E\psi_l \tag{12}$$

valid for $l=1,\ldots,N$ if we require the boundary conditions

$$\psi_0=\psi_{N+1}=0 \tag{13}$$

We define a local amplitude a_l and a local phase φ_l by

$$\begin{aligned}\psi_{l+1}&=a_l\sin(\varphi_l+\kappa)\\ \psi_l&=a_l\sin\varphi_l\end{aligned} \tag{14}$$

and require a_l to be positive. κ is at our disposal within $0<\kappa<\pi$. For the ordered case $\varepsilon_l\equiv 0$ one finds

$$\varphi_l=\varphi_0+l\kappa, \quad a_l=\text{const.} \tag{15}$$

with the choice

$$E=-2V\cos\kappa \tag{16}$$

The boundary conditions (13) read

$$\varphi_0=0 \bmod \pi, \quad \varphi_N=-\kappa \bmod \pi \tag{17}$$

Dividing (12) by ψ_l and using (14) we obtain the recursion relation

$$\begin{aligned}&\operatorname{ctg}\varphi_l-\operatorname{ctg}(\varphi_{l-1}+\kappa)\\ &=\left(\frac{\varepsilon_l-E}{V}-2\cos\kappa\right)/\sin\kappa\end{aligned} \tag{18}$$

Since a_l is positive the signs of $\sin\varphi_l$ and $\sin(\varphi_{l-1}+\kappa)$ are equal. If $\sin\varphi_l=0$ then ψ_{l+1} and ψ_{l-1} have opposite signs. Consequently $\sin(\varphi_l+\kappa)$ and $\sin\varphi_{l-1}$ have opposite sign in this case. Thus, for given φ_{l-1} the phase is determined *modulo* 2π.

3. One Boundary Condition

a) Phase Distribution

Suppose only the boundary condition $\varphi_0=0$ is given, whereas φ_N may be arbitrary. Then there is a solution for arbitrary E and the phase φ_r is given by $\varepsilon_1,\ldots,\varepsilon_r$. The probability distribution for the ε's may be converted into one for the φ's

$$dP_r = \prod_{l=1}^{r} (p(\varepsilon_l)\, d\varepsilon_l)$$
$$= \prod_{l=1}^{r} (p(\varepsilon_l)\, d\varphi_l) \left| \frac{\partial(\varepsilon_1, \ldots, \varepsilon_r)}{\partial(\varphi_1, \ldots, \varphi_r)} \right|$$
$$= \prod_{l=1}^{r} (K_0(\varphi_l, \varphi_{l-1})\, d\varphi_l) \tag{19}$$

where

$$K_0(\varphi_l, \varphi_{l-1}) = p(\varepsilon_l) \left| \frac{\partial \varepsilon_l}{\partial \varphi_l} \right|$$
$$= \frac{V \sin\kappa \cdot p(\varepsilon_l)}{\sin^2 \varphi_l} \tag{20}$$

Here ε_l is considered to be a function of φ_l and φ_{l-1} according to (18). If the condition below (18) is not fulfilled, then p is taken to be zero.
With the notation for the iterated kernel

$$K_0^r(\varphi_r, \varphi_0) = \prod_{l=1}^{r-1} \left(\int d\varphi_l\right) \prod_{l=1}^{r} K_0(\varphi_l, \varphi_{l-1}) \tag{21}$$

we obtain the probability density w_r for the phase φ_r

$$w_r(\varphi_r) = K_0^r(\varphi_r, \varphi_0) \tag{22}$$

For appropriate distributions $p(\varepsilon)$ the density w_r will converge to a limit distribution $w(\varphi)$ for $r \to \infty$ which obeys

$$w(\varphi) = \int d\varphi'\, K_0(\varphi, \varphi')\, w(\varphi') \tag{23}$$

b) Ratio of Amplitudes

Next consider the average $\langle (a_0/a_r)^n \rangle$. From (14) one expresses the ratio of the amplitudes by the phases

$$\frac{a_{l-1}}{a_l} = \frac{\sin\varphi_l}{\sin(\varphi_{l-1} + \kappa)} \tag{24}$$

Thus, with (19) we obtain

$$\langle (a_0/a_r)^n \rangle = \int \prod_{l=1}^{r} \left(\frac{\sin\varphi_l}{\sin(\varphi_{l-1} + \kappa)} \right)^n dP_r$$
$$= \int d\varphi_r K_n^r(\varphi_r, \varphi_0) \tag{25}$$

with

$$K_n(\varphi_l, \varphi_{l-1}) = \frac{V \sin\kappa\, p(\varepsilon_l)}{\sin^{2-n}\varphi_l \sin^n(\varphi_{l-1} + \kappa)} \tag{26}$$

For large r the average (25) will be dominated by the largest eigenvalue $\lambda_0^{(n)}$ of the equation $\lambda f = K_n f$, yielding

$$\langle (a_0/a_r)^n \rangle \sim \lambda_0^{(n) r} \tag{27}$$

Obviously one has $\lambda_0^{(0)} = 1$. Taking the derivative of (27) with respect to n at $n = 0$ yields

$$\langle \ln(a_0/a_r) \rangle \sim + r \frac{d\lambda_0^{(n)}}{dn} \tag{28}$$

From this expression we obtain the localization length ξ_0,

$$1/\xi_0 = \lim_{r \to \infty} \frac{1}{r} \langle \ln(a_r/a_0) \rangle = - \left. \frac{d\lambda_0}{dn} \right|_{n=0} \tag{29}$$

$(\psi_{r+1}^2 + \psi_r^2)^{1/2}$ in (1) differs from a_r by a factor depending on φ_r. Because of the factor $1/r$ in front of the expectation value it is negligible in the limit $r \to \infty$.

c) Properties of K and λ_0

The properties of K_n and its maximum eigenvalue $\lambda_0^{(n)}$ have been discussed in [7] and [8]. First we note the symmetry property

$$K_n(\varphi, \varphi') = K_{2-n}(-\kappa - \varphi', -\kappa - \varphi) \tag{30}$$

For a $p(\varepsilon)$ which is strictly positive within some interval there is a unique solution for the maximum eigenvalue $\lambda_0^{(n)}$ and the corresponding eigenfunction. The symmetry property (30) implies

$$\lambda_0^{(n)} = \lambda_0^{(2-n)} \tag{31}$$

The maximum eigenvalue of K_0 is unity, (13). We have

$$\lambda_0^{(0)} = \lambda_0^{(2)} = 1 \tag{32}$$

From the Schwarz' inequality one deduces

$$\lambda_0^{(n+\delta n)} \lambda_0^{(n-\delta n)} \geqq \lambda_0^{(n)2} \tag{33}$$

from which one concludes

$$\lambda_0^{(1)} \leqq 1, \qquad \lambda_0^{(-1)} \geqq 1 \tag{34a, b}$$

and

$$\xi_0^{-1} = - \left. \frac{d\lambda_0^{(n)}}{dn} \right|_{n=0} \geqq 0 \tag{35}$$

For truely disordered systems one shows by means of the theorem of Furstenberg [9], see [10], that the inequality sign in (35) holds. Kunz and Souillard [8] have given a much simpler proof for the inequality sign in (34a) and (35). Equations (34) and (35) imply together with (27) and (28) that the amplitudes increase in the average with increasing r.

4. Both Boundary Conditions Fulfilled

a) Averages

Now we require that both boundary conditions are fulfilled. The eigenenergies E_i depend on the energies $\varepsilon_1, \ldots, \varepsilon_N$, $E_i = E_i(\varepsilon)$. The number of eigenstates in the interval $E \ldots E + dE$ be $N\rho(E)\,dE$. Then the average $\langle f \rangle_E$ of a function $f(\psi)$ evaluated for the eigenstates $\psi^{(i)}$ in this energy interval is given by

$$N\rho(E)\langle f(\psi)\rangle_E = \int dP_N \sum_i f(\psi^{(i)})\,\delta(E - E_i(\varepsilon)) \tag{36}$$

$N\rho(E)$ is obtained from (35) from (35) by choosing $f = 1$. We transform

$$dP_N = \prod_{l=1}^{N} (p(\varepsilon_l)\,d\varepsilon_l)$$
$$= \prod_{l=1}^{N} p(\varepsilon_l) \left| \frac{\partial(\varepsilon_1, \ldots, \varepsilon_N)}{\partial(\varphi_1, \ldots, \varphi_{N-1}, E_i)} \right| \prod_{l=1}^{N-1} d\varphi_l\, dE_i \tag{37}$$

The Jacobian in this equation may be written

$$\pm \frac{\partial(\varepsilon_1, \ldots, \varepsilon_{r-1}, E_i, \varepsilon_{r+1}, \ldots, \varepsilon_N)}{\partial(\varphi_1, \ldots, \varphi_{r-1}, E_i, \varphi_r, \ldots, \varphi_{N-1})} \frac{\partial \varepsilon_r}{\partial E_i} \tag{38}$$

where the derivative $\partial \varepsilon_r / \partial E$ has to be taken so that all ε's save ε_r are fixed. Then $\partial E_i / \partial \varepsilon_r = |\psi_r^{(i)}|^2$. For fixed E_i the phases $\varphi_1, \ldots, \varphi_{N-1}$ depend only on $\varepsilon_1, \ldots, \varepsilon_{r-1}$. Similarly $\varphi_1, \ldots, \varphi_{N-1}$ depend only on $\varepsilon_{r+1}, \ldots, \varepsilon_N$. Thus, the Jacobian in (38) can be written

$$\frac{\partial(\varepsilon_1, \ldots, \varepsilon_{r-1}, E_i)}{\partial(\varphi_1, \ldots, \varphi_{r-1}, E_i)} \frac{\partial(\varepsilon_{r+1}, \ldots, \varepsilon_N)}{\partial(\varphi_r, \ldots, \varphi_{N-1})} \frac{1}{|\psi_r^{(i)}|^2} \tag{39}$$

The first Jacobian is a product of factors K_0, (19). Similarly one can show that the second Jacobian in (39) is a product of factors K_2. Putting all factors together one obtains

$$dP_N = dP_{r-1} \frac{p(\varepsilon_r)\,dE_i}{|\psi_r^{(i)}|^2} d\tilde{P}_r \tag{40}$$

with

$$d\tilde{P}_r = \prod_{l=r}^{N-1} (K_2(\varphi_{l+1}, \varphi_l)\,d\varphi_l) \tag{41}$$

For given phases φ and E_i there is only one set of ε's which obeys (18). Thus, the sum in (36) yields only one contribution after integration over E_i

$$N\rho(E)\langle f(\psi)\rangle_E = \sum_{\varphi_N} \int dP_{r-1} \frac{p(\varepsilon_r)}{|\psi_r|^2} d\tilde{P}_r\, f(\psi) \tag{42}$$

We choose $\varphi_0 = 0$. For φ_N we have to allow for the two choices $\varphi_N = -\kappa$ and $\varphi_N = \pi - \kappa$. This is meant by the sum over φ_N. Using that ψ_r is normalized, we may also write

$$N\rho(E)\langle f(\psi)\rangle_E = \sum_{r=1}^{N} \sum_{\varphi_N} \int dP_{r-1}\, p(\varepsilon_r)\, d\tilde{P}_r f(\psi) \tag{43}$$

dP_{r-1} is the probability distribution for a chain with boundary condition $\varphi_0 = 0$ and fixed energy E as discussed in Sect. 3. For large r it contains with high probability wavefunctions whose amplitudes increase from $l = 1$ to $l = r$. Similarly $d\tilde{P}_r$ is the probability distribution for a chain with boundary condition $\varphi_N = -\kappa \bmod \pi$ and fixed energy E. Thus, for large $N - r$ it contains with high probability wavefunctions whose amplitudes increase from $l = N$ to $l = r$. Thus, a typical eigenfunction increases from both ends up to site r where they are matched together (with the factor $p(\varepsilon_r)$). Finally the summation over all sites r has to be performed.

b) Density of States

From (43) we obtain the density of states

$$N\rho(E) = \sum_{r, \varphi_N} \int K_0^r(\varphi_r, \varphi_0) \frac{\sin^2 \varphi_r}{V \sin \kappa} \cdot K_2^{N-r}(\varphi_N, \varphi_r)\,d\varphi_r \tag{44}$$

For r and $N - r$ sufficiently large we use the limit w of K_0^r and similarly (compare (30))

$$\lim_{N-r \to \infty} K_2^{N-r}(\varphi_N, \varphi_r) = w(-\varphi - \kappa) \tag{45}$$

which yields for $N \to \infty$

$$\rho(E) = \frac{2}{V \sin \kappa} \int w(\varphi_r) \sin^2 \varphi_r\, w(-\varphi_r - \kappa)\,d\varphi_r \tag{46}$$

c) Correlations

We may also use (42) to calculate $\langle \psi_r \psi_{r'} \rangle_E$,

$$N\rho(E)\langle \psi_r \psi_{r'} \rangle_E = \sum_{\varphi_N} \int dP_{r-1} \frac{\psi_{r'}}{\psi_r} p(\varepsilon_r)\, d\tilde{P}_r \tag{47}$$

We choose ψ to be real. From (14) we obtain (for $r' > r$)

$$\frac{\psi_{r'}}{\psi_r} = \prod_{l=r}^{r'-1} \frac{\sin(\varphi_l + \kappa)}{\sin \varphi_l} \tag{48}$$

which yields with (26)

$$N\rho(E)\langle\psi_r\psi_{r'}\rangle_E$$
$$=\frac{1}{V\sin\kappa}\sum_{\varphi_N}\int d\varphi_r d\varphi_{r'} K_2^{N-r'}(\varphi_N,\varphi_{r'})$$
$$\cdot\sin\varphi_{r'} K_1^{r'-r}(\varphi_{r'},\varphi_r)\sin\varphi_r K_0^r(\varphi_r,\varphi_0) \tag{49}$$

which for large r and $N-r'$ reduces to

$$N\rho(E)\langle\psi_r\psi_{r'}\rangle_E$$
$$=\frac{2}{V\sin\kappa}\int d\varphi d\varphi' w(-\varphi'-\kappa)$$
$$\cdot\sin\varphi' K_1^{r'-r}(\varphi',\varphi)\sin\varphi w(\varphi) \tag{50}$$

K has two types of eigenfunctions, those with short period $f(\varphi+\pi)=f(\varphi)$ and alternating ones $f(\varphi+\pi)=-f(\varphi)$. $w(\varphi)$ is of short-period. Since $\sin\varphi$ is alternating only alternating eigenfunctions of K_1 contribute. Let us denote the largest eigenvalues of the alternating eigenfunctions by $\lambda_{\pm1}^{(1)}$. Then at large distances the correlation of ψ decays like

$$\langle\psi_r\psi_{r'}\rangle_E = c\,\lambda_1^{(1)|r'-r|}+c^*\,\lambda_{-1}^{(1)|r'-r|}. \tag{51}$$

λ_{-1} is the complex conjugate λ_1. If we write the correlation as a product of an oscillating term with an envelope

$$\langle\psi_r\psi_{r'}\rangle_E = |c|\cos(k|r-r'|)\,e^{-|r-r'|/\xi_1}, \tag{52}$$

then a phase coherence length ξ_1 is given by

$$|\lambda_1^{(1)}| = e^{-1/\xi_1}. \tag{53}$$

Similarly we evaluate

$$N\rho(E)\langle|\psi_r\psi_{r'}|\rangle_E$$
$$=\frac{2}{V\sin\kappa}\int d\varphi d\varphi' w(-\varphi'-\kappa)|\sin\varphi'|$$
$$\cdot K_1^{r'-r}(\varphi',\varphi)|\sin\varphi|\,w(\varphi) \tag{54}$$

and find

$$\langle|\psi_r\psi_{r'}|\rangle_E \sim \lambda_1^{(0)|r-r'|}\sim e^{|r-r'|/\hat{\xi}} \tag{55}$$

which defines a localization length $\hat{\xi}$,

$$|\lambda_1^{(0)}| = e^{-1/\hat{\xi}} \tag{56}$$

Here $\lambda_1^{(0)}$ is the largest eigenvalue of K_1 (for short-period eigenfunctions).

5. Weak Disorder

a) The Kernel K

Suppose there are only small fluctuations in ε and suppose the average of ε vanishes,

$$\langle\varepsilon\rangle=\int\varepsilon p(\varepsilon)\,d\varepsilon=0$$
$$\langle\varepsilon^2\rangle=\int\varepsilon^2 p(\varepsilon)\,d\varepsilon=\eta \tag{57}$$

We will now determine the various lengths ξ and the density of states in lowest order in η. For this purpose we consider

$$g(\varphi)=\int K_n(\varphi,\varphi')f(\varphi')\,d\varphi'$$
$$=\int p(\varepsilon)\left(\frac{\sin\varphi}{\sin(\varphi'+\kappa)}\right)^{n-2} f(\varphi')\,d\varepsilon \tag{58}$$

We notice that with (16) the recurrence relation (18) reads

$$\operatorname{ctg}(\varphi'+\pi)=\operatorname{ctg}\varphi-\hat{\varepsilon} \tag{59}$$

with

$$\hat{\varepsilon}=\varepsilon/(V\sin\kappa) \tag{60}$$

From (59) we obtain

$$\frac{\sin^2\varphi}{\sin^2(\varphi'+\kappa)}$$
$$=1-2\hat{\varepsilon}\cos\varphi\sin\varphi+\hat{\varepsilon}^2\sin^2\varphi \tag{61}$$
$$\varphi'=\varphi-\kappa+\hat{\varepsilon}\sin^2\varphi+\hat{\varepsilon}^2\sin^3\varphi\cos\varphi+o(\hat{\varepsilon}^3) \tag{62}$$

If we substitute (61), (62) into (58) and keep all terms in order $\hat{\varepsilon}^2$, then the integral equation (58) reduces to

$$g(\varphi)=f(\varphi-\kappa)+\hat{\eta}D_n f(\varphi-\kappa) \tag{63}$$

with

$$D_n=\left(\frac{n}{2}-1\right)\sin^4\varphi+\left(\frac{n}{2}-1\right)(n-3)\sin^2\varphi\cos^2\varphi$$
$$+(3-n)\sin^3\varphi\cos\varphi\frac{\partial}{\partial\varphi}+\tfrac{1}{2}\sin^4\varphi\frac{\partial^2\varphi}{\partial\varphi^2} \tag{64}$$

and

$$\hat{\eta}=\langle\hat{\varepsilon}^2\rangle=\eta/V^2\sin^2\kappa=4\eta/(4V^2-E^2) \tag{65}$$

A short calculation yields

$$D_n e^{im\varphi}=\sum_{n=-2}^{+2} c_{m+2k,m}^{(n)} e^{i(m+2k)\varphi} \tag{66}$$

with

$$c_{m\pm4,m}^{(n)}=-\tfrac{1}{32}(2-n\pm m)(4-n\pm m)$$
$$c_{m\pm2,m}^{(n)}=\tfrac{1}{8}(2-n\pm m)(1\pm m)$$
$$c_{m,m}^{(n)}=\tfrac{1}{16}(n^2-2n-3m^2) \tag{67}$$

b) Non-degenerate Perturbation Theory

For $\hat{\eta}=0$ the eigenvalue equation $\lambda f=Kf$ has the solutions

$$\lambda_m^{(n)}=e^{-im\kappa}, \quad f_m^{(n)}=e^{im\varphi} \tag{68}$$

For $\hat{\eta}\neq 0$ we may try the ansatz

$$\lambda_m^{(n)}=e^{-im\kappa}(1+\hat{\eta}\,\delta\lambda_m^{(n)}) \tag{69}$$

$$f_m^{(n)}=e^{im\varphi}(1+\hat{\eta}\,\delta f_m^{(n)}) \tag{70}$$

Substitution of (69), (70) into the eigenvalue equation and collecting all terms of order $\hat{\eta}$ yields

$$\delta\lambda_m^{(n)}+\delta f_m^{(n)}(\varphi)=\delta f_m^{(n)}(\varphi-\kappa)+e^{-im\varphi}\,D_n e^{im\varphi} \tag{71}$$

which with (66) yields

$$\delta\lambda_m^{(n)}=c_{m,m}^{(n)} \tag{72}$$

$$\delta f_m^{(n)}(\varphi)=\sum_k{}' \frac{c_{m+2k,m}^{(n)}}{2i\sin(k\kappa)}\,e^{ik(2\varphi+\kappa)} \tag{73}$$

where the sum runs over $k=-2,\ -1,\ +1,\ +2$. From the denominators in (73) it is apparent that this perturbation theory breaks down for $\sin\kappa=0$ and $\sin(2\kappa)=0$ that is at the original band edges $E=\pm 2V$ and in the centre of the band, $E=0$. At energies $0<|E|<2V$, however, (72) and (29), (53), (56) yield

$$\partial\lambda_0^{(n)}/\partial n=-\hat{\eta}/8, \quad \lambda_0^{(1)}=1-\hat{\eta}/16,$$
$$\lambda_1^{(1)}=e^{-i\kappa}(1-\hat{\eta}/4) \tag{74}$$

and thus

$$\hat{\xi}=\frac{16}{\hat{\eta}}, \quad \xi_0=\frac{8}{\hat{\eta}}, \quad \xi_1=\frac{4}{\hat{\eta}} \tag{75}$$

We note that for the Anderson model with a rectangular distribution of ε of width W one has $\eta=W^2/12$, thus with (65) the result by Thouless for ξ_0, (3), is obtained.

c) Degenerate Perturbation Theory

In the vicinity of $E=0$ one has to perform degenerate perturbation theory, since for $\kappa=\frac{\pi}{2}$ the eigenvalues $\lambda_m^{(n)}$, (69), of the unperturbed problem are highly degenerate. Let us expand f in the eigenfunctions for the unperturbed problem

$$f^{(n)}(\varphi)=\sum b_k e^{ik\varphi} \tag{76}$$

Substitution into the eigenvalue equation and collecting the terms proportional $e^{ik\varphi}$ yields

$$(\lambda-e^{-ik\kappa})\,b_k=\hat{\eta}\sum_{k'} c_{k,k'}^{(n)}\,e^{-ik'\kappa}b_{k'} \tag{77}$$

For $\lambda\approx e^{-im\kappa}$ and $\kappa\approx\frac{\pi}{2}$ the first factor on the left-hand side becomes small for $k=m+4l$, l integer. Thus, we keep all b's with index $m+4l$. The other b's are smaller by a factor $\hat{\eta}$. With (69) and

$$\kappa=\tfrac{\pi}{2}+\delta\kappa=\tfrac{\pi}{2}+\frac{E}{2V}, \quad x=\frac{\delta\kappa}{\hat{\eta}} \tag{78}$$

for small $\delta\kappa$ and E (77) reduces to

$$(\delta\lambda-4lix-c_{m+4l,m+4l}^{(n)})\,b_{m+4l}$$
$$=c_{m+4l,m+4l+4}^{(n)}\,b_{m+4l+4}+c_{m+4l,m+4l-4}^{(n)}\,b_{m+4l-4} \tag{79}$$

This set of equations can be solved easily numerically. One chooses $b_m=1$ and iterates (79) for b_{m+4l} (if $l\neq 0$) and for $\delta\lambda$ if $l=0$. We observe that $\delta\lambda$ and the eigenfunctions depend on x only, which for the Anderson model yields (7). The lengths ξ and the density of states are plotted in Figs. 1a to 1d. The values for $E=0$ are listed in Table 1. The derivative $\partial\lambda_0^{(n)}/\partial n$ for $n=0$ is obtained from (79) for $m=l=0$.

$$\delta\lambda=c_{0,0}^{(n)}+c_{0,4}^{(n)}b_4+c_{0,-4}^{(n)}b_{-4}$$
$$=n\left[\frac{n}{16}-\frac{1}{8}-\frac{1}{32}(n+2)(b_4+b_{-4})\right] \tag{80}$$

Thus

$$\left.\frac{\partial\delta\lambda_0^{(n)}}{\partial n}\right|_{n=0}=\left.-\frac{1}{8}-\frac{1}{16}(b_4+b_{-4})\right|_{n=0} \tag{81}$$

The density of states is obtained from (46). We have

$$w(\varphi)=\frac{1}{2\pi}f_0^{(0)}(\varphi) \tag{82}$$

which obeys the normalization condition

$$\int_0^{2\pi} w(\varphi)\,d\varphi=1 \tag{83}$$

with $b_0=1$. Since only the b_{4l}, l integer contribute for $\hat{\eta}\to 0$ and x fixed we obtain

$$2\pi V\rho(E)=\sum_{l=-\infty}^{\infty} b_{4l}^2 \tag{84}$$

d) Approximate Solution

An approximate solution can be obtained by solving (79) for $b_{m\pm 4}$ neglecting $b_{m\pm 8}$ and approximating $\delta\lambda$ by (72)

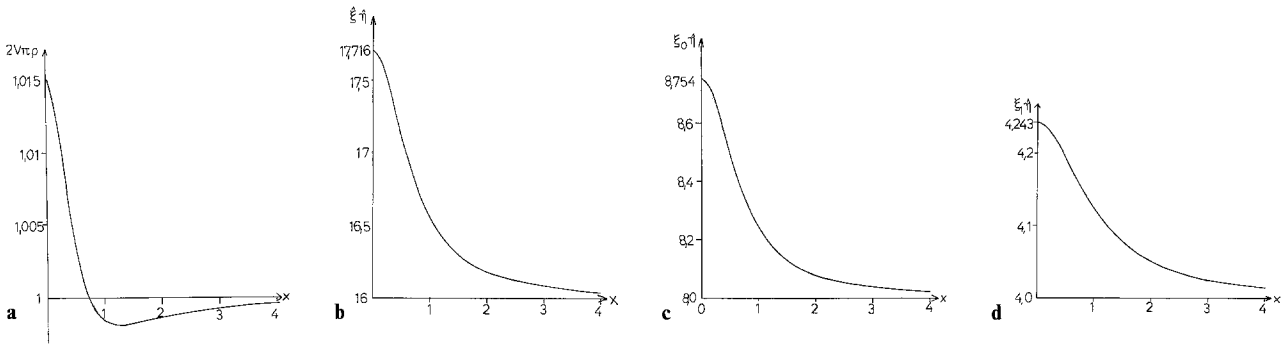

Fig. 1a–d. The density of states and the lengths $\hat{\xi}$, ξ_0, and ξ_1 as a function of x

$$b_{m\pm4}=\frac{c_{m\pm4,m}}{c_{m,m}-c_{m\pm4,m\pm4}-4ix} \tag{85}$$

In a second step (85) is substituted in (79) for $l=0$ which yields

$$\delta\lambda_m^{(n)}=c_{m,m}^{(n)}+c_{m,m+4}^{(n)}b_{m+4}+c_{m,m-4}^{(n)}b_{m-4} \tag{86}$$

Thus, we obtain the approximation

$$\frac{\partial}{\partial n}\delta\lambda_0\bigg|_{n=0}=-\frac{1}{8}+\frac{3/32}{9+16x^2}$$

$$\delta\lambda_0^{(1)}=-\frac{1}{16}+\frac{27/512}{9+16x^2}$$

$$\delta\lambda_1^{(1)}=-\frac{1}{4}+\frac{1/16}{9/2-4ix}$$

$$2\pi V\rho=1+\frac{9-16x^2}{8(9+16x^2)^2} \tag{87}$$

The values of this approximation at the band centre are given in Table 1. One can easily check that these expressions (87) are correct in order x^{-2} in an expansion in powers of x^{-1}. The corresponding asymptotic expressions for ξ and ρ are given in Table 1.

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