AD-A094 966 PRINCETON UNIV N J DEPT OF PHYSICS F/G 20/10
THE THOULESS CONJECTURE FOR A ONE-DIMENSIONAL CHAIN.(U)
JAN 81 P W ANDERSON, P A LEE N00014-77-C-0771

UNCLASSIFIED

1 OF 1
AD
AD 94966

END
DATE
FILMED
3-81
DTIC

The Thouless Conjecture for a One-Dimensional Chain

P. W. Anderson and P. A. Lee
Bell Laboratories
Murray Hill, New Jersey 07974

ERRATUM

Equation (13) of this paper does not follow from (12). The correct Equation (13) is:

$$\phi_{1,2} = \theta \pm \cos^{-1} (|r| \cos \phi).$$

The remainder of the paper is completely unaffected.

THE THOULESS CONJECTURE FOR A ONE-DIMENSIONAL CHAIN

by

P. W. Anderson* & P. A. Lee

Bell Laboratories

Murray Hill, N.J. 07974

ABSTRACT

The Thouless conjecture relating energy level shifts as a function of boundary conditions to conductance is shown to be incorrect in detail in the one-dimensional chain, though qualitatively correct: the dimensionless conductances defined by scattering theory and by Thouless' conjecture are functions of each other.

*Also at Princeton University, Princeton, N.J. 08544
The work at Princeton University was supported in part by the National Science Foundation Grant No. DMR 78-03015, and in part by the U.S. Office of Naval Research Grant No. N00014-77-C-0711.

THE THOULESS CONJECTURE FOR A ONE-DIMENSIONAL CHAIN

P. W. Anderson* and P. A. Lee

Bell Laboratories

Murray Hill, New Jersey 07974

D. Thouless[1] has proposed a relationship between quantum conductivity of an electron system, density of states, and a parameter describing the average sensitivity of state energies to boundary conditions. We give his argument shortly.

In the course of a detailed study, using the scattering theory of conductance, of scaling of the conductance in a 1d chain system[2], we tried to demonstrate explicitly the connection proposed by Thouless. We did indeed find that the conductance G is a function of Thouless' parameter

$$g_T = \frac{<\delta E>}{<\Delta E>} \tag{1}$$

where n(E), the density of states, is $< 1/\Delta\ E >$ and $<\delta\ E>$ is a geometric mean of the energy level shifts caused by a reversal of the phase of the boundary conditions from periodic to antiperiodic. (This reversal is along the direction of current flow: in other, transverse, directions the boundary conditions are considered irrelevant so long as they are kept fixed). But for this particular case, the function seems to differ from that proposed by Thouless, i.e., to be proportional to the square, not the first power.

Thouless gives two arguments for this relationship, both rather heuristic and relying on macroscopic limits: one from the Kubo formula and one a rather qualitative one based on the uncertainty principle. We give the latter which is, to our minds, more convincing. (A recent study of the Kubo formula[3] shows that it contains localization information in a rather obscure form, and must be handled with care.)

We imagine a wave-packet of electrons started off on one side of a block of material of

* Also at Princeton University, Princeton, New Jersey 08544 Work at Princeton University was supported in part by the National Science Foundation Grant No. DMR 78-03015, and in part by the U. S. Office of Naval Research Grant No. N00014-77-C-0711.

length L. In so far as the material has a conductivity, at some length scale $L >> l_{atomic}$ the wave-packet will exhibit classical diffusive behavior, we suppose. At first this diffusion takes place as though the other side of the block were nonexistent, and independently of boundary conditions; but after diffusion to the other end, one will begin to see a difference in the reflection of the diffused packet depending on boundary conditions, i.e., at a time

$$t_D = \frac{L^2}{D} \tag{2}$$

where D is the diffusion constant.

What happens at time t_D can be assumed, by the uncertainty principle, to involve energy level changes $\hbar\delta\omega \sim 1/t_D$. Thus it is supposed that

$$<\delta E> \simeq \hbar/t_D \simeq \frac{\hbar D}{L^2}.$$

By the Einstein relationship - in this case a trivial balancing of conduction versus diffusion currents in the presence of an electric field - we derive

$$\sigma = e^2 D \frac{dn}{dE}$$

but in a sample of size L^d, d the dimensionality,

$$\frac{dn}{dE} = <\frac{1}{\Delta E}> L^d$$

so that

$$<\delta E> <\frac{1}{\Delta E}> \cong \frac{\hbar\sigma}{e^2} L^{d-2} \cong \frac{\hbar G}{e^2} \tag{3}$$

(3) is what we have called the Thouless conjecture.

Neither the uncertainty principle argument about energy levels nor the macroscopic, statistical limit defining t_D is quite rigorous, so we attempted to verify Eq. (3) in a system we think can solve exactly, the 1d linear random chain. In this system a nearly rigorous theory of conductivity exists based on the scattering theory definition of conductance,

$$G = \frac{e^2}{\pi\hbar} T/R \tag{4}$$

where T and R are the quantum *reflection* and *transmission* coefficients of the sample considered as a scatterer of 1d waves along a channel, considered to be connected to perfectly transmitting, infinite reservoirs to left and right (see Fig. 1). Eq. (4) does not contain any eigenvalue information, but the S-matrix which determines T and R is related to the eigenvalue problem under periodic boundary conditions because it also determines the "transfer matrix" M which relates wave-function amplitudes at left and right hand ends of the sample. A second way in which S is related to energy eigenvalues is that the density of states in a given length of chain is equal to $\frac{1}{2\pi}$ times the rate of change in the scattering phase-shifts with energy. Putting these two relations together, it turns out we can relate the eigenvalue spectrum to the magnitudes of t and r.

Let us now make these relationships precise. The scattering matrix S may be written in terms of the in-going and out-going channels on left and right, i_L, i_R, o_L, o_R, as

$$o = \underset{\sim}{S}\, i \tag{5}$$

with

$$S = \begin{pmatrix} r & t \\ t & r' \end{pmatrix} \tag{6}$$

(We confine ourselves to time-reversal invariant scatterers for which S is symmetric: $\underset{\sim}{S} = \underset{\sim}{\tilde{S}}$)

so that

$$\begin{aligned} o_L &= r i_L + t i_R \\ o_R &= t i_L + r' i_R \end{aligned} \tag{5a}$$

(see Fig. 1). In Eq. (4) $T = |t|^2$ and $R = |r|^2 = |r'|^2$. Eq. (5a) can be solved for the amplitudes in the R channels in terms of the L ones

$$R = M\ L \qquad \begin{pmatrix} i_R \\ o_R \end{pmatrix} = M \begin{pmatrix} o_L \\ i_L \end{pmatrix} \tag{7}$$

Here we have chosen the representation so that diagonal channels represent waves going in the same direction, for reasons which will become clear.

Solving (5a) for i_R, o_R, we get

$$M = \begin{pmatrix} \frac{1}{t} & -\frac{r}{t} \\ \frac{r'}{t} & t - \frac{rr'}{t} \end{pmatrix}$$

Here it is useful to use unitarity of the S-matrix to simplify. Unitarity gives, of course,

$$|r|^2 + |t|^2 = |r'|^2 + |t|^2 = 1$$

but also the orthogonality relation is

$$rt^* + tr'^* = 0;$$

i.e.,

$$\frac{r}{t} = -\frac{r'^*}{t^*}$$

$$\text{(and also } \frac{r'}{t} = -\frac{r^*}{t^*}\text{)}$$

so that

$$t - \frac{rr'}{t} = t + \frac{|r|^2}{t^*} = \frac{1}{t^*}. \tag{8}$$

Thus

$$M = \begin{pmatrix} \frac{1}{t} & -\frac{r}{t} \\ -\frac{r^*}{t^*} & \frac{1}{t^*} \end{pmatrix} \tag{9}$$

Note that M is Hermitian in the sense that $M^* = M$ with diagonal elements interchanged. This is adequate to ensure diagonalizability with a unitary transformation.

Eigenvalues of the periodic problem in which the scatterer S is repeated can be calculated by inserting the inputs of M into its outputs, i.e.,

$$M\psi = \lambda\psi.$$

The eigenvalues of M are the solutions of

$$\left(\frac{1}{t} - \lambda\right)\left(\frac{1}{t^*} - \lambda\right) = \left|\frac{r}{t}\right|^2$$

$$\lambda = \mathrm{Re}\,\frac{1}{t} \pm \sqrt{\left(\mathrm{Re}\frac{1}{t}\right)^2 - 1} \tag{10}$$

Thouless' formula can be applied in two different versions: one may relate the conductance either to the energies of two "band edge" points at which

$$\lambda = \pm 1, \ \mathrm{Re}\frac{1}{t} = \pm 1$$

(Corresponding to periodic and antiperiodic boundary conditions) or to the "effective mass curvature" at the edge of the band $\frac{\partial^2 E}{\partial \eta^2}$ obtained by setting

$$\lambda = e^{i\eta} \quad \eta << 1. \tag{11}$$

Before discussing these quantities, let us work out the other relationship, that between E and the eigenvalues $e^{i\phi_i}$ of S. Here ϕ_i are the two scattering phase shifts which must characterize a two-by-two S matrix. To calculate these

$$(r - e^{i\phi_i})\,(r' - e^{i\phi_i}) = t^2$$

$$e^{2i\phi_i} - e^{i\phi_i}(r+r') + rr' - t^2 = 0$$

Again, we use the unitarity relations (8):

$$e^{2i\phi_i} - e^{i\phi_i}(r+r') - \frac{t}{t^*} = 0$$

or

$$e^{2i\phi_i} - e^{i\phi_i}(r+r') + \frac{r'^*}{r} = 0 \tag{12}$$

If we write

$$r = |r|e^{i(\theta+\phi)};\ r' = |r|e^{i(\theta-\phi)}$$

we find that

$$\phi_1 = \theta + \phi \quad \phi_2 = \theta - \phi; \tag{13}$$

as is not unexpected: the two phase shifts are those of the two reflected waves. As it must be, the sum of the phase shifts

$$\phi_1 + \phi_2 = 2\theta$$

is representation invariant: ϕ is determined by the choice of origin, but

$$\frac{1}{\pi} <\frac{\partial\theta}{\partial E}> = n(E),$$

the density of states contained in the scatterer, (for spherical scatterers this is the Friedel[4] theorem) so θ must be an invariant. This is also closely related to the transmission phase shift by

$$\frac{r}{r'^*} = e^{2i\theta} = -\frac{t}{t^*} = e^{2i\psi+\pi}$$

$$\theta = \psi + \frac{\pi}{2} \tag{14}$$

where

$$t = |t|e^{2i\psi} \tag{15}$$

Thus also

$$<\frac{\partial\psi}{\partial E}> = \pi n(E) \tag{16}$$

Now we are in a position to derive the relationship. We note that $\frac{\partial\psi}{\partial E}$ is non-negative (otherwise it would never be a suitable density of states, and also there is a theorem of scattering theory) while $|t|$ cannot vanish (see Ref. 2), and is ≤ 1, in fact, in all reasonable cases < 1. Thus 1/t follows a path rotating constantly outside the unit circle in the complex plane as a function of energy, and if we are already in the scaling region where fairly large numbers of incoherent scatterers are present, and the region contains many wavelengths, $<|t|>$ doesn't vary as we traverse very many circuits so any amplitude increase must be followed by a decrease and vice versa. In fact, we have verified that the distribution of $|t|$

calculated elsewhere[2] would not lead to a substantial effect on the Thouless conjecture. We therefore assume $|t|$ constant and calculate the energy shifts as a function of θ. That is,

$$\frac{\delta E}{\Delta E} \simeq \frac{\delta\psi}{\pi} \tag{17}$$

since there are two states for every rotation of 2π. $\delta\psi$ is the angular shift defined by either of the two methods:

$$(\delta\psi)_{p-a} = \psi_{\lambda=-1} - \psi_{\lambda=+1}$$

or

$$(\delta\psi)_{curvature} = 2\frac{\delta^2\psi}{\delta\eta^2} \tag{18}$$

with η defined in Eq. (11). We have now that

$$\lambda = \pm 1$$

implies that

$$\mathrm{Re}\frac{1}{t} = \pm 1$$

$$\frac{\cos\psi}{|t|} = \pm 1$$

$$(\delta\psi)_{pa} = 2\sin^{-1}|t| \tag{19}$$

For small t this is equivalent to

$$\sin\psi\ \delta\psi = 2|t|$$

$$\delta\psi = \frac{2t}{\sin\psi} = 2\frac{|t|}{\sqrt{1-|t|^2}}$$

$$= 2\left|\frac{t}{r}\right|$$

Similarly, evaluating $\frac{\delta^2\psi}{\delta\eta^2}$ (10) gives

$$\frac{\cos\psi}{t} = \mathrm{Re}(\frac{1}{t}) = \cos\eta$$

$$\frac{\sin\psi\delta\psi}{|t|} = \frac{\eta^2}{2}$$

$$\frac{\delta^2\psi}{\delta\eta^2} = \frac{|t|}{\sin\psi}$$

$$(\delta\psi)_{curvature} = 2|\frac{t}{r}| \tag{20}$$

Remarkably, from (4), (19) and (20) we find that

$$G = \frac{e^2}{2\pi\hbar}(\frac{\delta E}{\Delta E})^2 \quad ! \tag{21}$$

(Using the curvature definition which Thouless remarks is more exact for large G; for the one involving sign change in the boundary conditions (20) fails for rather special 1-dimensional reasons in this extreme limit.) It is clear that Thouless' conjecture is *qualitatively* borne out, that is $\delta E/\Delta E$ is a good measure of the dimensionless conductance, going through unity at the crossover from local to extended; but the detailed numerical correlation is not right. This is not serious in the local limit (the localization length differs by a factor 2 only) but is disturbing in the extended one where one could expect the diffusion arguments to work.

The one-dimensional chain is a very special case and we see no obvious reason why these results should apply directly to real systems quasimacroscopic in more than one dimension. In particular, the eigenvalues of S obey much the same rules for a large system, but the eigenfunctions of M and those of S are not at all the same - they are related by a random unitary transformation in channel space. It is not clear how the motions of the two sets of eigenvalues are related to each other. It is surprising but true that 1d localization of G is almost precisely comparable in the two cases[5]; but the same need not be true of the Thouless conjecture.

[It is a pleasure to submit a paper to a volume in honor of my old friend, Ryogo Kubo. Among the many valuable things I learned long ago from him was the important lesson that today's formal, mathematical results may lie at the heart of tomorrow's physics; it is in this spirit I submit this. PWA]

REFERENCES

(1) J. T. Edwards and D. J. Thouless, J. Phys. C. 802 (1972); D. J. Thouless, les Houches Lectures, 1978.

(2) P. W. Anderson, D. J. Thouless, E. Abrahams, D. S. Fisher, Phys. Rev. B, (to be published in October).

(3) S. Kirkpatrick and D. J. Thouless, preprint.

(4) J. Friedel, Adv. in Phys. 3, 446 (1954); for a more general discussion, see M. I. Goldberger and K. M. Watson, *Collision Theory* (New York, 1964).

(5) We have under preparation a manuscript of the many-channel, 1d system repeating the methods of Ref. (2) in this case.

Figure Captions

Fig. 1: Resistive sample as a scatterer

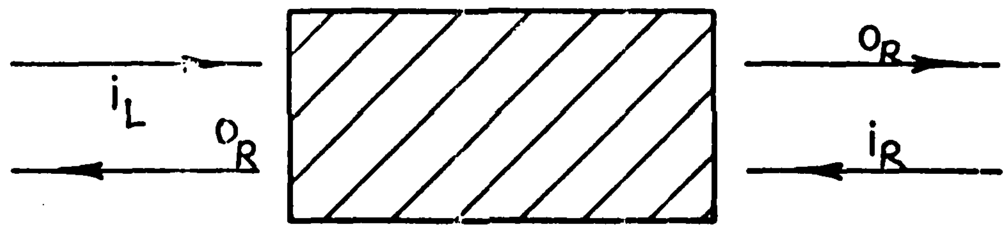

Fig. 1

UNCLASSIFIED

SECURITY CLASSIFICATION OF THIS PAGE (When Data Entered)

REPORT DOCUMENTATION PAGE

READ INSTRUCTIONS BEFORE COMPLETING FORM

1. REPORT NUMBER	2. GOVT ACCESSION NO. AD-A094 966
3. RECIPIENT'S CATALOG NUMBER	
4. TITLE (and Subtitle) The Thouless Conjecture for a One-Dimensional Chain	5. TYPE OF REPORT & PERIOD COVERED technical report 1980 Preprint
	6. PERFORMING ORG. REPORT NUMBER
7. AUTHOR(s) P.W. Anderson*and P.A. Lee*	8. CONTRACT OR GRANT NUMBER(s) N00014-77-C-0711
9. PERFORMING ORGANIZATION NAME AND ADDRESS Department of Physics, Princeton University Princeton, N.J. 08544 *also Bell Laboratories, Murray Hill, U.J. 07974	10. PROGRAM ELEMENT, PROJECT, TASK AREA & WORK UNIT NUMBERS NR 318-058
11. CONTROLLING OFFICE NAME AND ADDRESS Office of Naval Research (Code 427) Arlington, Va. 22217	12. REPORT DATE January 21, 1981
	13. NUMBER OF PAGES 9 + 1 Figure
14. MONITORING AGENCY NAME & ADDRESS(if different from Controlling Office)	15. SECURITY CLASS. (of this report) Unclassified
	15a. DECLASSIFICATION/DOWNGRADING SCHEDULE

16. DISTRIBUTION STATEMENT (of this Report)

Approved for public release; distribution unlimited.

17. DISTRIBUTION STATEMENT (of the abstract entered in Block 20, if different from Report)

18. SUPPLEMENTARY NOTES

Prog. Theor. Physics

19. KEY WORDS (Continue on reverse side if necessary and identify by block number)

one dimension
localization

20. ABSTRACT (Continue on reverse side if necessary and identify by block number)

The Thouless conjecture relating energy level shifts as a function of boundary conditions to conductance is shown to be incorrect in detail in the one-dimensional chain, though qualitatively correct: the dimensionless conductances defined by scattering theory and by Thouless' conjecture are functions of each other.

DD FORM 1 JAN 73 1473 EDITION OF 1 NOV 65 IS OBSOLETE
S/N 0102-LF-014-6601

UNCLASSIFIED

SECURITY CLASSIFICATION OF THIS PAGE (When Data Entered)

LMED

8