Revisiting Thouless conductance formula

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Abstract

It was shown using perturbation theory[1] that Thouless energy $E_c$ for a quantum system scales linearly with the conductance of the system. We derive in an alternate way in 1-D that $E_c$ scales with the conductance in a very different way. We physically show the difference between our approach and that of ref. 1 to expect our results to hold in higher dimensions also. We verify our results with exact numerical calculations.

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Quantum mechanical (electron) transport through disordered system has been of great importance for quite a long time. A major simplification of the problem was conceived by Landauer when he proposed that although resistance is an outcome of dissipation and breakdown of time reversal symmetry one can formulate resistance in terms of elastic scattering only if one assumes a clear spatial separation between elastic processes and inelastic processes[2]. The so called Landauer’s conductance formula is now on firm grounds and is at the heart of studying transport through mesoscopic systems experimentally as well as theoretically[3]. Another important idea was put forward by Thouless[1]. According to him extended states are very sensitive to twisting of boundary conditions and also contribute highly to conductance. Whereas localized states are not so sensitive to twisting of boundary conditions and also contribute very little to conductance. So there must be a relation between conductance and a characteristic energy scale of the system called Thouless energy Ec. In his original work[1] Ec is defined as the average change in the eigen-energies of the system if we twist the boundary conditions from periodic to anti-periodic. Ec so defined appears to be a very artificial energy scale but it was latter found to be the typical inverse diffusion time[4]. This energy scale appears as a bridge to our understanding of universality from Anderson localization to Quantum chaos, universal conductance fluctuations[5], persistent currents[6,7] and many more. Using perturbation theory it was shown that Ec scales linearly with conductance[1] in the diffusive regime. In the localized regime in all dimensions (including 1D) Ec was found to be zero. However as Thouless relation is only for a finite sample (for an infinite sample average level spacing Δ goes to zero) there is no need to rule out the possibility of a relation between Ec and the conductance G even in the localized regime, i.e., when the localization length is much smaller than the sample length. The fact that Ec turns out to be zero when using perturbation theory is due to a particular approximation as stated in ref. 1. In this treatment we find a way to avoid this approximation in 1D and thus we find a scaling between Ec and G in the localized regime. In fact the relation derived here is general to all regimes (ballistic, diffusive and localized). Again diffusive regime in 1D means the localization length is much larger than the sample
Recent experiments on persistent currents has made it necessary to re-examine the Thouless formula critically[7]. In ref. 1 unless we appeal to Kubo Greenwood formula in 3D the results are true in all dimensions. One can just as well appeal to Landauer’s conductance formula in 1D. The fact that the scaling between $E_c$ and $G$ may not be linear in 1D when transmission is very small was first pointed out by Anderson and Lee[8]. But this work starts from the eigenvalues of the S matrix and M matrix and not from the eigen-functions and eigenvalues of the Hamiltonian as in ref.1 and hence it is not obvious whether it is a specialty of 1D as stated in ref. [8]. Recent work[9] however shows that $E_c$ is linearly related to $G$ as claimed in ref 1. We start from the eigen-functions and so the difference with ref. 1 is evident. Hence we can argue physically to expect our results to hold in higher dimensions also. We find that the scaling in 1D to the first order is same as that of Anderson and Lee. We write down all higher order terms in terms of the actually measurable two probe conductance and so in our case transmission need not be small. Our result is general to all three regimes.

As we have already mentioned that unless one appeals to Kubo formula in 3D the treatment of ref. 1 is identical in all dimensions we start by repeating its steps in 1D. Let there be a system of size $L$ with a random potential $V(x)$ defined by the Hamiltonian $H$ and the eigen-functions $\phi(x)$ satisfy periodic boundary conditions. This means $\phi(x)$ is the eigen-function of an infinite periodic potential formed by the repetition of the sample of length $L$. Change in boundary condition is equivalent to a gauge transformation such that the wave function

$$\psi(x) = \phi(x)e^{i\alpha x}$$

(1)

where $\phi(x)$ satisfy periodic boundary condition and satisfies the Schrodinger equation with additional terms $\alpha^2 + 2\alpha p_x$, where $p_x$ is the momentum operator. As $\phi(x)$ satisfy periodic boundary condition anti-periodic boundary condition for $\psi(x)$ is obtained by putting $\alpha L = \pi$ and periodic boundary condition for $\psi(x)$ is obtained by putting $\alpha L = 0$. 

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So $\alpha^2 + 2\alpha p_x$ can be treated as a perturbation to the Hamiltonian with periodic boundary conditions whose eigen-functions are $\phi(x)$ and thus $E_c$ can be calculated according to its original definition. However the shift is identified with the lowest order non-zero term in the perturbative expansion. We call this lowest order term $E_{c_l}$ and

$$E_{c_l} = \alpha^2 + 2\alpha \sum_j |[p_x]_{ij}|^2 \frac{E_i - E_j}{E_i - E_j}$$  \hspace{1cm} (2)

Here $[p_x]_{ij}$ are the matrix elements of $p_x$ between $\phi(x)$. Ref. 1 assumes these terms to be exponentially small and this assumption makes $E_{c_l}$ go to zero in the localized regime. However $\phi(x)$ is not an eigen-function of a random potential but the eigen-function of an infinite periodic potential formed by the repetition of the sample of length $L$. Hence $\phi(x)$ is not an exponentially decaying localized state but an extended Bloch state however random $V(x)$ is. Hence the neglected terms are not exponentially small but are reasonably large. We shall soon discuss that the difference can be as large as 100 times the actual value. After this one can relate $E_{c_l}$ to the conductance through Kubo Greenwood formula (in the diffusive regime) through the matrix elements of $p_x$. However in Kubo formula the matrix elements of $p_x$ is calculated between wave-functions of the system with open boundary conditions (coupled to a bath) to account for dissipation[9,10]. Hence these states are not extended Bloch states for a random $V(x)$ as that in eqn (2). Besides the approximation (used in ref. [1]) of the diffusive spectra being uncorrelated is not appropriate[9,11].

We start from eigen-functions given in eqn(1) and this allows us to express $E_c$ in terms of conductance.

$$\psi(x + L) = \phi(x + L)e^{i\alpha(L+x)}$$  \hspace{1cm} (3)

Now $\phi(x)$ is the eigen-function of a periodic potential and satisfies periodic boundary conditions. So we can write $\phi(x + L) = \phi(x)$ and thus we explicitly take care of the fact that the states are extended Bloch states. Hence

$$\psi(x + L) = \phi(x)e^{i\alpha x}e^{i\alpha L} = \psi(x)e^{i\alpha L}$$  \hspace{1cm} (4)

Now as a consequence of Bloch’s theorem[12] we can get eqn 19 of ref 7.
\[ \alpha L = \cos^{-1} re[1/t(E)] \] (5)

Where \( t(E) \) is the transmission amplitude at an incident energy \( E \), \( E \) being the eigen-energy corresponding to the Bloch eigen-function \( \phi(x) \). RHS of eqn 5 is the phase of the wave-function of the Bloch state. This could not be realized in ref. 7. When the conductor becomes perfectly ordered eqn 5 becomes \( \alpha L = kL \), \( k \) being the momentum. In presence of disorder eqn 5 is just \( \alpha L = KL \) \( K \) being the Bloch momentum, the state \( E \) being an extended state. This is exact for any arbitrary \( V(x) \) and we do not have to consider ballistic, diffusive or localized regime separately.

We can write \( re[1/t(E)] = \frac{\cos(\beta)}{|t|} \) where \( \beta \) is the transmission phase. Then we can take \( \cos(\beta) = \cos \frac{2\pi E}{\Delta} \). For a clean system where the dispersion is \( E \equiv k^2 \) this is exact. Except in the limit of extremely strong disorder this assumption is fairly accurate[13,14]. Now the bound-states of the system can be easily found using the periodic and anti-periodic boundary conditions.

The bound states \( E_n^p \) for the periodic boundary condition is obtained by putting \( \alpha = 0 \), i.e.,

\[ \cos^{-1} \left( \frac{\cos \frac{2\pi E}{\Delta}}{|t(E)|} \right) = 0 \] (6)

and the bound-states \( E_n^{ap} \) for the anti-periodic boundary condition is obtained by putting \( \alpha = \pi/L \), i.e.,

\[ \cos^{-1} \left( \frac{\cos \frac{2\pi E}{\Delta}}{|t(E)|} \right) = \pi \] (7)

and solving eqns 6 and 7 for \( E \). Hence the bound-states for the periodic boundary condition are

\[ \frac{2\pi E_n^p}{\Delta} = \cos^{-1} |t(E_n^p)| \] (8)

The bound-states for the anti-periodic boundary condition are

\[ \frac{2\pi E_n^{ap}}{\Delta} = \cos^{-1} (- |t(E_n^{ap})|) \] (9)
Then we use the expansion \[\frac{\pi}{2} - \cos^{-1}(y) = y + \frac{1}{2.3}y^3 + \frac{1.3}{2.4.5}y^5 + \frac{1.3.5}{2.4.6.7}y^7 + \ldots \text{ for } y^2 \leq 1 \] (10)

to obtain

\[
2\pi \frac{|E_n - E_{ap}^n|}{\Delta} = (|t(E_n^p)| + |t(E_{ap}^n)|) + \frac{1}{2.3}(|t(E_n^p)|^3 + |t(E_{ap}^n)|^3) + \\
\frac{1.3}{2.4.5}(|t(E_n^p)|^5 + |t(E_{ap}^n)|^5 + \ldots) \tag{11}
\]

Now Landauer’s conductance formula gives the dimensionless conductance \(g(E)\) as

\[
g(E) = |t(E)|^2 \tag{12}
\]

Now we can take the average of both sides of (11) over disorder configuration. In 1D where we do not have a mobility edge it is appropriate to take an arithmetic mean of the LHS. It is also appropriate to take the arithmetic mean of the RHS because \(|t(E)|\) is less than unity. Thus we get \(Ec/\Delta\) in terms of dimensionless conductance \(g(E)\) as given by Landauer’s formula. Note that \(<|t(E_n^p)|>=<|t(E_{ap}^n)|>\) because modulus of transmission do not depend on the phase of the wave function.

\[
\frac{Ec}{\Delta} = 1/\pi(<\sqrt{g(E)}>) + \frac{1}{2.3} <\sqrt{g(E)}>^3 + \frac{1.3}{2.4.5} <\sqrt{g(E)}>^5 + \ldots \tag{13}
\]

We have nowhere invoked the condition that transmission is small. It shows to a leading order Thouless energy depends on \(<\sqrt{g(E)}>\) and not \(<g(E)>)\ as obtained in ref. [8]. Thouless energy \(Ec\), i.e., the average energy difference between a periodic and anti-periodic system is a fundamental energy scale governing transport in a quantum system. \(Ec\) that appears in eqn. 13 is not just the shift given by the first order perturbation but is the shift if all higher order terms are taken into account. We can relate this fundamental energy scale to the conductance. This may shed light on the nature of transport in a random medium more accurately.
However the shift as given by the lowest order perturbation term i.e., $E_{cl}$ can be very accurately calculated from the curvature of energy versus $\alpha L$ dispersion curve at $\alpha L=0$. Subsequently we find the scaling between $E_{cl}$ and $g$. From eqn 5

$$\cos \frac{2\pi E}{\Delta} = |t(E)| \cos(\alpha L)$$  \hspace{1cm} (14)

For small $\alpha L$

$$\frac{2\pi E}{\Delta} = \cos^{-1}[|t(E)| \cdot w]$$  \hspace{1cm} (15)

where $w = 1 - (\alpha L)^2/2 + (\alpha L)^4/4 + ....$. Again using the expansion given in eqn 10 we find

$$\frac{2\pi E}{\Delta} = \pi/2 - |t(E)| - \frac{1}{2.3} |t(E)|^3 - \frac{1.3}{2.4.5} |t(E)|^5 - .... + |t(E)| \left( \frac{(\alpha L)^2}{2} + \frac{1}{2.3} |t(E)|^3 \frac{3(\alpha L)^2}{2} + \frac{1.3}{2.4.5} |t(E)|^5 \frac{5(\alpha L)^2}{2} + .... \right)$$

$a', b'$, etc. are functions of $|t(E)|$ whose explicit forms we do not need to know.

Then using (12) and taking average of both sides over different disorder configurations one finds

$$\frac{2\pi}{\Delta} \left. \frac{d^2 E}{d(\alpha L)^2} \right|_{(\alpha L)=0} \frac{2\pi}{\Delta} E_{cl} = \sqrt{g(E)} + (\sqrt{g(E)})^3/2 + (\sqrt{g(E)})^5/2.4 + ....$$  \hspace{1cm} (17)

Again we find that to a leading order $E_{cl}$ goes as $\sqrt{g}$ and not as $g$. As we can write down all higher order terms our expression is valid for entire range of $|t|$. This is the extra benefit of our alternate derivation. Ref [1] underestimates the shift because the eigenstates used in the perturbative calculations were not taken as Bloch states. As soon as we imply periodic boundary condition we impose a discrete symmetry in the system that results in making the eigenstates of the system extended Bloch states however strong the disorder is.

Recent experiments on persistent currents support this. Magnetic field can be taken as a physical realization of $\alpha L$ and persistent currents (averaged over disorder and summed...
over levels) arising due to sensitivity of eigenstates to twisting of boundary condition can be taken as a measure of Ec. Ref. [7] is the only theory known so far that gives the magnitude of persistent current correct to an order of magnitude. Ref [7] shows that in a ring with radial grain boundaries states are Bloch states. In such a situation disorder can suppress conductance 100 times more than it suppresses persistent currents. Whereas in a ring with point defects states are localized and then disorder suppresses persistent currents by the same amount it suppresses conductance. When one calculates the ratio between two numbers the proportionality constants do not matter at all but the scaling matters. This suggests localized states will show linear scaling between Ec and G and the treatment of Thouless goes through.

In higher dimensions if we start with periodic boundary conditions in all three directions (as is the original definition of Ec) then we imply the same discrete symmetry as in 1-D and the states are extended. Twisting boundary condition in one direction will shift the states more than that given by perturbation theory. However in higher dimension we do not know a simple expression for Bloch states in terms of conductance as in (5). One can numerically study these situations although one may have to resort to more complicated averaging procedures.

This result is expected to hold for the tight binding model also although the coefficients can change a lot. In the continuum model average Δ as well as average conductance monotonically increase with energy but not in the tight binding model. These will change the coefficients drastically but the same type of scaling of Ec with g should be there. This we verify numerically. Also in the limit of extremely strong disorder Δ approximately goes as W/N[14] where W is the strength of the disorder and N is the number of sites. Hence the above equation can be extended to the regime of extreme strong disorder too.

To verify numerically for a tight binding chain we take a chain consisting of 15 sites. We find its eigenvalues for periodic as well as anti-periodic boundary conditions by exact numerical diagonalization. We arrange the eigen values in ascending order and then calculate average Ec/Δ. Then we average over 100 disorder configurations. < √g > is also evaluated
exactly using transfer matrix method, and then averaging over 100 configurations. In fig (1) we show that \( \frac{E_c}{\Delta} \) depends on \( < \sqrt{g} > \) in a way that can be best fitted to a polynomial of the type given in eqn (13). A minimum of three terms are needed to give a reasonable fit suggesting the importance of higher order terms. In fig. (2) we show that \( \frac{E_c}{\Delta} \) versus \( < \sqrt{g} > \) cannot be fitted to a power law curve although the power in the best fit is close to one is very suggestive. Also a fit to a general polynomial of three terms is much worse than the fit in fig. (1) if one keeps in mind that after all it is a three parameter fit. Other type of fits also do not work. We have left out the extreme strong disorder limit where the fit deteriorates. However one can study this regime with the modification explained before.

Hence Thouless argument leading to eqn. (13) and (17) will give the conductance as that given by Landauer’s conductance formula in all three regimes of 1D. \( E_c I \) and \( \Delta \) can be calculated using diagonalization techniques and in some cases eqn. (17) may be easier to deal with. It may specially simplify the problem of treating the effect of e-e interaction on conductance.

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FIGURE CAPTIONS

Fig. 1. Plot of Ec/Δ versus $<\sqrt{g}>$ shown by dots. Solid line is the best fit to a polynomial of the type given in eqn. (13) which is $y=1.84691x - 2.9037x^3 + 2.04372x^5$.

Fig. 2. Plot of Ec/Δ versus $<\sqrt{g}>$ shown by dots. Solid curve 1 is the best fit to a power law curve which is $y=.902978x^{1.1292}$. The solid curve 2 is the best fit to a general polynomial of three terms which is $y=4.81251x - 9.62012x^2 + 5.78701x^3$. 

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