Anomalies in the transport properties of a disordered solid

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(Received 23 August 1983; revised manuscript received 17 October 1983)

This paper points to the existence of new anomalies in the transport properties of a one-dimensional solid. The anomalies are associated with the period-($r \geqslant 2$) marginally stable cycles of a key-phase recurrence relation. Standard perturbation theory diverges at these points and an alternative expansion about the periodic cycles is introduced. The low-order anomalies corresponding to $r=2$ and 3 are evaluated.

It is well known[1–5] that the spectral and localization properties of disordered solids contain anomalies that are absent in their crystalline counterparts. The most notable of these arise at a band center, where for particular models[4–7] the density of states can diverge. For such models the anomalies are known to be a consequence of a symmetry of the Hamiltonian. However, anomalies also arise in the absence of such symmetries.[1,8,9] An example is provided by the Anderson model with unit hopping elements and random site energies of mean-square deviation σ^2. Thouless[10] has shown that the inverse localization length α at a band center takes the form $\alpha=\sigma^2/4+O(\sigma^4)$, whereas Kappus and Wegner[1] find that the exact result is $\alpha=\sigma^2/C+O(\sigma^4)$, with $C=4.377\ldots$. This discrepancy is due to the presence of a sharp band center resonance in α of width $\sim\sigma^2$.

In the present paper it is noted that the band center anomaly is just one of an infinite set of resonances arising within an energy band. The resonances correspond to the periodic marginally stable cycles of a finite difference equation for the phase ϕ of a real solution of the Schrödinger equation. To each cycle there is a corresponding anomaly in the random system, the band center anomaly being associated with the period-2 cycle. Within a band in the zero-noise limit there are an infinite number of such cycles and as a consequence nondegenerate perturbation theory diverges everywhere. To evaluate a given anomaly a theory is described which incorporates an expansion about the cycles of interest and, for a particular model, anomalies at the period-2 and -3 cycles are evaluated explicitly.

Following Schmidt[11] and Landauer,[12] the integrated density of states per scatterer $D(E)$ and the inverse localization length α are conveniently computed within a random T-matrix approach,[13] which yields the general result

$$\alpha-2\pi iD(E)=\alpha_1+\alpha_2-2i\theta\ , \tag{1}$$

where

$$\theta=\langle\theta_j\rangle,\ \alpha_1=-\langle\ln(1-S_j^2)\rangle$$

and

$$\alpha_2=2\langle\ln(1+S_j\exp[i(\theta_j-\theta_j'+\phi_{j-1})])\rangle\ . \tag{2}$$

The quantities S_j,θ_j,θ_j' approaching in the above equations are a dimensionless scattering parameter and phases associated with the T matrix of the jth scatterer and are readily calculated within a given model.[13]

Equation (1) is a realization of a result due to Thouless[14] and Herbert and Jones[15] that the inverse localization length and integrated density states are real and imaginary parts of the same complex number. The quantities α_1 and θ on the right-hand side are readily evaluated, because they involve known quantities only. The problem of computing α and $D(E)$ is reduced to that of evaluating the remaining contribution α_2. This involves an average over the cumulative phase ϕ, which is found to satisfy the following recurrence relation,[13]

$$\exp[i\phi_j]=\frac{\exp[i(\theta_j+\phi_{j-1})]+S_j\exp[i\theta_j']}{\exp[-i\theta_j]+S_j\exp[i(\phi_{j-1}-\theta_j')]}\ . \tag{3}$$

The anomalies under consideration arise in the weak-disorder, weak-scattering limit, where $S_j \ll 1$. In this limit, Eq. (2) yields

$$\alpha_2=2a_{101}\mu_1-a_{202}\mu_2+\tfrac{2}{3}a_{303}\mu_3+\cdots\ , \tag{4}$$

where the following notation has been employed,

$$\mu_m=\langle\exp[im\phi_j]\rangle\ ,$$

$$a_{pqr}=\langle S_j^p\exp[i(q+r)\theta_j+i(q-r)\theta_j']\rangle\ ,$$

and it has been noted that, for a one-dimensional solid, ϕ_{j-1} is independent of the nature of the jth segment.

A simple "nondegenerate" perturbation theory which yields a series for the moments μ_m will be illustrated by evaluating α_2 to lowest order in S. Expanding Eq. (3) to first order in S and averaging yields

$$\mu_1(1-a_{011})=a_{110}-a_{112}\mu_2\ .$$

Similarly, squaring and averaging yields $\mu_2(1-a_{022})=O(S)$. Hence in the limit $S\to 0$, provided $a_{011}\neq 1$ and $a_{022}\neq 1$, one obtains

$$\mu_1=a_{110}/(1-a_{011})$$

and

$$\alpha_2=2a_{101}a_{110}/(1-a_{011})\ . \tag{5}$$

It is straightforward to extend the analysis to higher order in S. However, more conditions of the form $a_{orr}\neq 1$ are thereby generated. For a given energy, one or more of these conditions will be violated and, at some high order in S, the perturbation series will diverge.

To illustrate this, consider a sequence of equal strength delta functions with positions x_j uniformly distributed over the interval $\pm\Delta x$ centered at their crystalline values ja. For this model the quantities S_j and θ_j are independent of the disorder, so the subscripts will be omitted. One obtains

$$a_{pqr}=S^P\sigma_{q-r}\exp[i(q+r)\theta]\ ,$$
$$\theta=K_0a-\arctan[S/(1-S^2)^{1/2}]\ , \tag{6}$$

where

$$\sigma_m=(\sin 2mK_0\Delta x)/2mK_0\Delta x$$

and K_0 is the Fermi wave vector. For such a system, Fig. 1 shows the variation of α with θ when $S=0.22$, $\Delta x=1$, and the electron energy $=1$ eV. The top graph ($\alpha=$ constant) shows the result of combining Eqs. (16) and (11) to yield α to order S^2. The center figure shows the result of evaluating α to order S^4, while in the bottom figure, terms up to order S^6 have been evaluated. As higher-order terms are computed, an increasing number of divergences arise which eventually populate the whole of an energy band. Such divergences are clearly unphysical. They can be attributed to the presence of periodic cycles in Eq. (3) (Ref. 16) and signal the appearance of anomalies in α and $D(E)$. In what follows, the low-order in-band anomalies in α will be evaluated.

In the zero-noise limit, it is clear from the connection between the integrated density of states and the phase change per scatterer[11] that a period-1 attractor must occupy an interval corresponding to an energy gap. This interval is marked in Fig. 1. The divergence of perturbation theory as a band edge is crossed can hardly be regarded as anomalous, so that in what follows, we focus attention on the period-($r\geq 2$) cycles only. The position θ_r of a period-r cycle is given by[16]

$$\cos\theta_r=(1-S^2)^{1/2}\cos m\pi/r,\quad m=1,2,\ldots,r-1\ . \tag{7}$$

Within a band, these values of θ form a dense set of measure zero.

The general problem of computing the moments μ_m close to a given cycle can be solved by constructing the "degenerate" counterpart of the above nondegenerate perturbation theory. Raising both sides of Eq. (3) to an arbitrary power m, expanding in S, and averaging yields a "secular" equation of the form

$$\sum_{p=1}^{\infty} W_{mp}\mu_p=a_{mmo}\ , \tag{8}$$

where

$$W_{mp}=\delta_{mp}-\sum_{(k\geq m-p)}^{m}(-1)^{k+p-m}\times\frac{m!(k+p-1)!}{(m-k)!k!(k+p-m)!}a_{2k+p-m,m,p}\ .$$

Within a band in the presence of noise it is readily shown that $\lim_{m\to\infty}\mu_m=0$. Hence the sum on the left-hand side of Eq. (8) can be cut off at some large value of P ($=P_c$ say) to yield a simple matrix equation for the moments. In practice, α_2 is computed for a given choice of P_c and then recomputed for a larger choice until convergence is achieved. To this end it is useful to expand about the cycle of interest by writing $\theta=\theta_r+\xi_r$. It is also convenient to introduce the parameter $\nu_r=\xi_r/S^2(1-\sigma_1^2)$ which embodies the noncommutability of the limits $S\to 0$, $\Delta x\to 0$, and $\xi_r\to 0$.

As an example, consider the period-2 anomaly at a band center where $\theta_2=\pi/2$. To lowest order in S, the earlier expression for μ_1 in terms of μ_2 remains valid, so an expression for μ_2 yields α_2 to lowest order. Choosing $P_c=2$, one obtains from (8) $\mu_2=\beta/(1-i\nu_2)$, where $\beta=(\sigma_1^2-\sigma_2)/4(1-\sigma_1^2)$. Similarly, choosing $P_c=4$ yields

$$\mu_2=\frac{\beta}{1-i\nu_2-\dfrac{9\beta^2/2}{1-i\nu_2/2}}\ . \tag{9}$$

This simple approximation contains the essential features of the result for α shown in Fig. 2, obtained by inverting Eq. (8) with $P_c=8$. Shown also in Fig. 2 are the results of a numerical simulation in a sequence of 10^6 delta functions.

The analysis at a period-3 cycle follows a similar pattern. The anomaly arises via the moment μ_3 and affects α_2 at order S^4. Choosing $P_c=4$ yields

$$\mu_3\sim\frac{O(S)}{1-i\nu_3[2\sqrt{3}/(3\sqrt{3}+i)]}\ .$$

Similarly, the result obtained by inverting Eqs. (8) with $P_c=8$ is shown in Fig. 3.

Note that the vertical axes of Figs. 2 and 3 differ by orders of magnitude. To understand the scaling behavior of successive anomalies, it is sufficient to note that the rth anomaly affects α_2 through the moment μ_r. As $\nu_r\to\infty$ this quantity is of order S^r, whereas when $\nu_r\to 0$, μ_r is of order

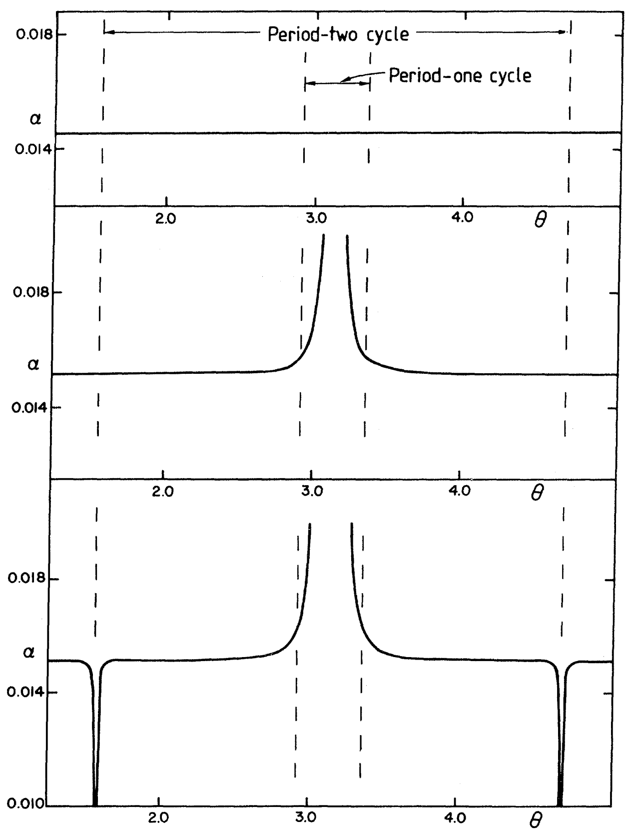

FIG. 1. Result for α obtained by employing nondegenerate perturbation theory to evaluate Eq. (4) to order S^2 (top), S^4 (center), and S^6 (bottom). As higher-order terms are included, an increasing number of divergences arise.

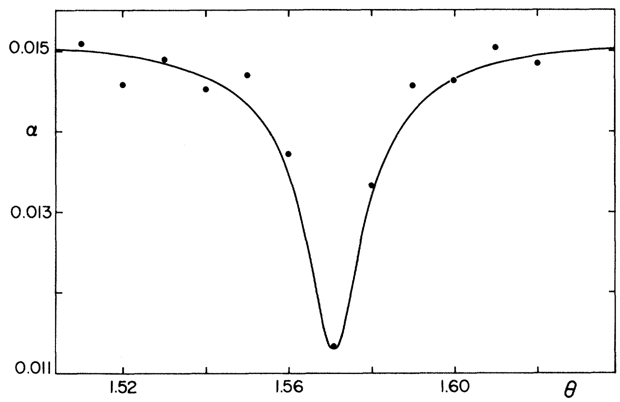

FIG. 2. Band center period-2 anomaly in α, obtained by inverting the matrix W of Eq. (8) with $P_c=8$. For comparison, the dots show the results of a numerical simulation carried out along the lines described in Ref. 12 on a sequence of 10^6 scatterers. No improvement is obtained by increasing P_c.

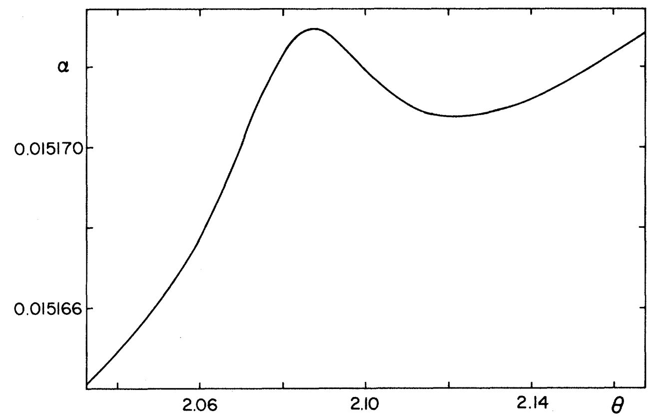

FIG. 3. Period-3 anomaly in α obtained from Eq. (8) with $P_c=8$. The peak position is given accurately by the denominator of Eq. (9).

S^{r-2}. Hence from the expansion (4) one obtains, for the relative magnitude of the anomaly at a period-r cycle, $\alpha_2(0)=\alpha_2(\infty)=O(S^{2r-2})$, where we have written $\alpha_2=\alpha_2(\nu)$. This shows that the weight under a resonance decreases exponentially with the periodicity of the associated cycle.

It is to be emphasized that these resonances are not simply an artifact of the delta-function model. The formalism leading to Eqs. (5) and (8) can be applied to a variety of one-dimensional disordered systems. In particular, Eqs. (1) to (5) yield for the Anderson model discussed in the introduction, $\alpha_1=\langle s^2\rangle+O(\sigma^4)$ and $\alpha_2=-\mu_2\langle s^2\rangle+O(\sigma^4)$, where $\langle s^2\rangle=\sigma^2/(4-E^2)+O(\sigma^4)$. To lowest order at a band center ($E=0$) the contribution $\alpha_1=\sigma^2/4$, which is simply Thouless's result for the inverse localization length α. The anomaly arises from the contribution α_2, which may be obtained from μ_2. To compute this quantity, one again proceeds from Eq. (8) by expanding about the period-2 cycle. The results are identical to those of the delta-function model (Eq. 9) provided the symbols are redefined as follows: $\nu_2\rightarrow 4\xi_2/3\sigma^2$, $\beta\rightarrow\frac{1}{12}$. Thus the resonances arising within these two different models have essentially the same shape. Choosing $P_c=2$ yields, for the parameter C introduced in the opening paragraph, $C=4.364\ldots$. Similarly, choosing $P_c=4$ yields $C=4.376\ldots$.

It has been shown that nondegenerate perturbation theory contains spurious divergences, which signal the presence of anomalies in the transport properties of a one-dimensional disordered solid. The anomalies can be computed by expanding about the periodic cycles of a cumulative phase ϕ and appear to be a general feature of one-dimensional disordered chains. It has been noted that the period-($r\geqslant 2$) cycles of the zero-noise map for ϕ are marginally stable. Some insight into the origin of the anomalies can be gained by examining the question of how these can be stabilized. From the connection between $D(E)$ and the phase change per scatterer,[11] it is clear that a *stable* cycle at a given energy is accompanied by a gap in the density of states. Hence, for example, the application of a symmetry-breaking term, which displaces every second scatterer of the crystal and effectively doubles the lattice constant, should stabilize the band center cycle. Such symmetry breaking leads to fine structure in the transport properties of the resulting crystal, which evidently survives in the presence of noise. The present paper does not address the question of whether or not the anomalies persist to higher dimensions. However, the presence of a band center resonance in at least one model of a two-dimensional disordered solid[7] suggests that the answer will be in the affirmative.

ACKNOWLEDGMENTS

I wish to thank M. F. Thorpe and P. Beale for useful discussions, and the United Kingdom Science and Engineering Research Council for the provision of a research fellowship.

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