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LOW ENERGY DENSITY OF STATES FOR DISORDERED CHAINS

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Résumé.- Nous calculons exactement la limite basse énergie pour la densité d'états de chaînes linéaires à couplage aléatoire entre premiers voisins. Nos résultats peuvent être appliqués aux vibrations du réseau d'une chaîne à constantes élastiques aléatoires ; à la diffusion de particules classiques avec des taux de transfert aléatoires ; et aux bandes électroniques liaison forte avec désordre corrélé diagonal et non-diagonal.

Abstract.- We calculate exactly the low energy limit for the density of states of linear chains with random near-neighbor coupling. Our results are applicable to lattice vibrations of a chain with random force constants ; diffusion of classical particles with random transfer rates ; low lying spin wave states of the random Heisenberg chain ; and tight binding electron bands with correlated diagonal and off-diagonal disorder.

1. INTRODUCTION.- The purpose of this paper is to present exact results for the low energy limit of the density of states for random one dimensional systems. Our results will be useful for the determination of low temperature specific heats ; autocorrelation functions at long times, and estimates of the localization of excitations for low energy states. We exhibit exact results for these quantities for random one dimensional systems which generate eigenvalue equations of the Töplitz type :

$$-W_{n,n-1} X_{n-1}^\epsilon + (\epsilon + W_{n,n-1} + W_{n,n+1}) X_n^\epsilon - W_{n,n+1} X_{n+1}^\epsilon = \delta(n). \tag{1}$$

We shall be interested in situations where the W are random variables distributed independently according to a probability distribution $\rho(W)$. Physical systems which fall into this category are : a) lattice vibrations of a linear chain with random force constants /1/ ; b) diffusion of classical particles with random transfer rates /2/ ; c) low lying spin wave states for the random linear Hiesenberg chain /3/ ; and d) tight binding bands for electrons with correlated diagonal and off-diagonal disorder /4/.

2. MATHEMATICAL FORMALITIES.- The detailed mathematical techniques will be described in detail elsewhere /5/. Summarizing, we calculate the statistical average of X_0^ϵ . One has, for a definite distribution of W, the result

$$X_0^\epsilon = (\epsilon + g_1^\epsilon + g_{-1}^\epsilon)^{-1} \tag{2}$$

where

$$g_n^\epsilon = W_{n-1,n} [1 - (X_n^\epsilon / X_{n-1}^\epsilon)] \tag{3}$$

with g_n^ϵ obeying the iterative equations

$$g_n^\epsilon = [(1/W_{n,n+1}) + 1/(g_{n+1}^\epsilon + \epsilon)]^{-1} \tag{4}$$

From Eq. 4, the probability distribution for g_n^ϵ , $f^\epsilon(g)$, obeys the integral equation

$$f^\epsilon(g) = \int dg' f^\epsilon(g') dW \rho(W) \delta[g - \{1/W + 1/(g' + \epsilon)\}^{-1}] \tag{5}$$

This allows us to write the statistical average of X_0^ϵ as

$$\langle X_0^\epsilon \rangle = \iint dg f^\epsilon(g) dg' f^\epsilon(g') (\epsilon + g + g')^{-1} \tag{6}$$

For a large class of distributions $\rho(W)$, and for small ϵ , the leading contribution to integrals such as equation 6 is given correctly by replacing $f^\epsilon(g)$ by a delta function :

$$f^\epsilon(g) \approx \delta(g - \langle g \rangle^\epsilon), \quad \epsilon \rightarrow 0 \tag{7}$$

where $\langle g \rangle^\epsilon$ is the solution of

$$\epsilon = (\langle g \rangle^\epsilon + \epsilon)^2 \int dW \rho(W) (W + \langle g \rangle^\epsilon + \epsilon)^{-1} \tag{8}$$

Clearly, the small ϵ behavior of equation 1 is dominated by the behavior of $\rho(W)$ near $W = 0$. We consider three cases.

3. DENSITY OF STATES.- (a) $\lim_{W \rightarrow 0} \rho(W) = 0$. One can

define

$$\langle 1/W \rangle = \int \rho(W) dW/W \quad (9)$$

so that, from equation 8, to leading order

$$\langle g \rangle^\epsilon = \epsilon^{1/2} \langle 1/W \rangle^{-1/2} \quad (10)$$

(b) $\lim_{W \rightarrow 0} \rho(W) = \text{constant}$. To leading order, this results in

$$\langle g \rangle^\epsilon = (\epsilon / |\lambda_n \epsilon|)^{1/2} \quad (11)$$

(c) $\rho(W)$ diverges as $W \rightarrow 0$, but is integrable. We set

$$\rho(W) = W^{-\alpha}, \quad \alpha < 1 \quad (12)$$

with a suitable cutoff for normalization purposes. This distribution leads to

$$\langle g \rangle^\epsilon = \epsilon^{1/(2-\alpha)} \quad (13)$$

One notes that for all three cases one has

$\langle g \rangle^\epsilon \gg \epsilon$ as $\epsilon \rightarrow 0$, so that

$$X_0^\epsilon = [\langle g \rangle^\epsilon]^{-1} \quad (14)$$

In all three cases cited above, X_0^ϵ is the diagonal element of a Green's function. The density of states is the inverse Laplace transform of the inverse Laplace transform of X_0^ϵ . For lattice vibrations, for example, ω^2 plays the role of ϵ , so that one obtains for the "phonon" density of states for case (b)

$$N(\omega) \propto |\lambda_n \omega|^{1/2}, \quad (15)$$

while for case (c)

$$N(\omega) \propto \omega^{-\alpha/(2-\alpha)} \quad (16)$$

In other cases, the relevant density of states is proportional to $[\langle g \rangle^\epsilon]^{-1}$. We see that the low energy density of states is enhanced compared to the usual one dimensional behavior. This must reflect the localization of the small ϵ eigenstates on account of the presence of small transfer rates W .

4. LOCALIZATION OF EXCITATIONS.- Because of the appearance of W in the definition of g_n^ϵ (equation 3), one cannot determine easily the spatial extent of the eigenfunctions. Consider, for example, case (c) above. For this situation, X_n^ϵ is the Laplace transform of the occupation probability of site n at time t when site 0 was occupied at $t = 0$. One finds

$$X_0(t) \propto t^{-(1-\alpha)/(2-\alpha)} \quad (17)$$

Moreover, the $X_n(t)$ are monotonic at all times :

$$X_n(t) < X_m(t), \quad |n| < |m|, \quad (18)$$

Thus, the width of the spatial distribution of oc-

cupations must obey the inequality

$$\langle \sum_n |n| X_n(t) \rangle \gtrsim t^{(1-\alpha)/(2-\alpha)} \quad (19)$$

This sets a lower limit on the extension of the eigenfunctions for $\epsilon \sim 1/t$. That is, we find

$$\sum_n |n| \phi_\epsilon^2(n) \gtrsim \epsilon^{-(1-\alpha)/(2-\alpha)} \quad (20)$$

where $\phi_\epsilon(n)$ is the eigenfunction at site n for energy ϵ .

5. CONCLUSION.- We have shown how the low energy density of states and the spatial localization of eigenfunctions in random linear chains governed by equation 1 can be calculated for essentially arbitrary probability distributions. We have (briefly) discussed the associated time development of the excitation amplitude at the initial and spatially separated sites at subsequent times. One dimensional systems with random site-site couplings are known /6/ so that our conclusions may be of direct relevance to experiment.

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- /4/ Governed by the Hamiltonian

$$H = - \sum_n \{ [V_{n-1,n} + V_{n,n+1}] c_n^+ c_n + V_{n,n+1} [c_n^+ c_{n+1} + \text{h.c.}] \}$$
 where the c_n are on site Fermion operators, and the V_n are random.
- /5/ Reference 2 and to be published by the same authors.
- /6/ An example is quinolinium (TCNQ)₂. See Azevedo, L.J., and Clark, W.G., Phys. Rev. B16 (1977) 3252