Transport and localization amongst coupled substructures

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The dynamics of the transport of the mean-square diffuse wave amplitude among coupled substructures is examined. Applications include coupled quantum dots, reverberation rooms, and chaotic billiards. A self-consistent theory is found to predict classical diffusive behavior at strong coupling, but to predict localization when coupling times are comparable to or greater than Heisenberg times. Predictions are compared to an exact result, to the Vollhardt-Wolfle self-consistent theory for multiply scattering continua, and to direct numerical simulations.

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I. INTRODUCTION

The diffuse flow of wave energy between complex coupled subsystems is of concern in reverberation room acoustics and the structural acoustics of built systems. It is also relevant to coupled chaotic microwave cavities [1,2] and other optical devices and to arrays of quantum dots in the noninteracting electron regime [3]. For the flow of vibrational and acoustic energy in complex built structures one often [see especially the theory of statistical energy analysis (SEA) [4]] invokes an appealing analogy with heat transport and models this flow as diffusive. In such a picture it is imagined that coupling between substructures is sufficiently weak that the field in each substructure achieves an internal uniformity before it dissipates or leaks into other substructures; thus, the field in each substructure is presumed fully diffuse. It follows that energy transport rates are independent of details of the system's excitation and structure, and energy balance equations may be written that are independent of those details. It is correspondingly thought that SEA is valid if coupling rates between substructures are sufficiently weak compared to equilibration rates within substructures. As described elsewhere [5], however, if transport rates are slow compared to the spacing between modes [alternatively, if Thouless time (t_{Th}=time for diffusion across a system) is greater than Heisenberg time (t_{H}= inverse mean eigenfrequency spacing)], then transport behavior is qualitatively different from that predicted by the diffusion model. Modes and energy flows are localized; a source in one substructure deposits an energy (more properly mean square field, or quantum probability) which remains in the vicinity of that substructure, regardless of the amount of time allowed for flow.

For the special case of two equal-sized substructures (we henceforth term them "rooms" in an allusion to reverberation room acoustics) and in the limit of coupling weak compared to the spacings between modes, it was shown in [5] that the fraction of energy in the second room following a transient addition of energy to the first room asymptotes at late times at a steady-state value of order $\sqrt{c\sigma}$. In the stated limit this is much less than the value (1/2) expected by equipartition. Here c is modal density, $c=dN/d\omega$, and σ is initial leaking rate. The fraction of energy in the second room was furthermore found to initially grow at a classical rate and then overshoot its late-time value before finally relaxing to its steady state. This prediction was confirmed in numerical simulations and in laboratory experiments. Quantitative predictions were confined to the special case of two weakly coupled statistically identical substructures; however, the qualitative reasoning that predicts localization for small $c\sigma$ is presumed to apply to more arbitrary systems consisting of multiple substructures coupled with arbitrary strength. The work reported here is part of an effort to compose a theory for such systems.

It is also part of an effort seeking a more comprehensive understanding of Anderson localization in disordered structures in general by studying the dynamics of flow in localizing systems. That flow dynamics is critical for evaluating laboratory experiments in multiply scattering classical wave systems is well appreciated. To date there appears to be but one theory for that dynamics. That Vollhardt and Wolfle's self consistent theory of localization [6] has implications for flow dynamics has recently been emphasized [7]. Its predictions have compared well with numerical simulations [8].

The next section provides a brief review of the exact results obtained earlier for a two-room system at weak coupling. It is followed by an exposition of a more general theory for localization and transport in discrete systems and some applications.

II. EXACT RESULTS FOR A WEAKLY COUPLED PAIR OF SUBSTRUCTURES

Exact results for mean-flow dynamics are scarce. One such is for the case of two weakly coupled substructures. In [5] this was described by the model

$$-i\partial_t \mathbf{u} = [\mathbf{H}_1 + \mathbf{H}_2 + \mathbf{v}]\mathbf{u} + \mathbf{s}\delta(t), \tag{1}$$

where $\mathbf{H}_1$ and $\mathbf{H}_2$ are stochastic Hamiltonians for the different rooms; their sum is block diagonal. The partial Hamiltonians were taken to have (real, random) modes ϕ and ψ:

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$$\mathbf{H}_1\psi^n = \omega_n\psi^n, \quad \mathbf{H}_2\phi^\nu = \alpha_\nu\phi^\nu,$$

$$\psi^n \cdot \psi^m = \delta_{mn}, \quad \phi^\nu \cdot \phi^\mu = \delta_{\mu\nu}, \quad \phi^n \cdot \psi^m = 0, \tag{2}$$

with random eigenfrequencies ω and α. The coupling $\mathbf{v}$ was taken to be purely off block diagonal:

$$\phi^\nu \cdot \mathbf{v}\phi^\mu = \psi^n \cdot \mathbf{v}\psi^m = 0, \quad \phi^\nu \cdot \mathbf{v}\psi^n = \psi^n \cdot \mathbf{v}\phi^\nu = V_{n\nu}. \tag{3}$$

The source $\mathbf{s}$ acts in room No. 1 only:

$$\mathbf{s} \cdot \phi^\nu = 0; \quad \mathbf{s} \cdot \psi^n = s_n. \tag{4}$$

The total "energy" in the system is the sum of the energies in each room and is a constant:

$$E = \mathbf{u}^* \cdot \mathbf{u} = E_1 + E_2 = \sum_m |\mathbf{u} \cdot \psi^m|^2 + \sum_\mu |\mathbf{u} \cdot \phi^\mu|^2 = \sum_m s_n^2. \tag{5}$$

The model is imagined to describe two substructures, within each of which propagation is either ballistic and chaotic [1,2] or diffusive without localization.

The solution of Eq. (1) was taken in the form

$$\mathbf{u} = \sum_m a_m(t)\psi^m + \sum_\mu b_\mu(t)\phi^\mu, \tag{6}$$

and coupled ordinary differential equations were derived governing the coefficients a and b:

$$-i\partial_t a_n(t) = \omega_n a_n(t) + \sum_\mu V_{n\mu}b_\mu(t) + s_n\delta(t),$$

$$-i\partial_t b_\mu(t) = \alpha_\mu b_\mu(t) + \sum_\mu V_{n\mu}a_n(t). \tag{7}$$

On expanding a and b to leading order in powers of the presumed small quantity V, a procedure that is valid only at short times, and averaging over the stochastic quantities $V_{n\mu}$, it was shown that the energy in room 2 increases at a simple rate:

$$E_2 = \left\langle \sum_\mu |b_\mu(t)|^2 \right\rangle = 2\pi c_2\langle V^2\rangle Et, \tag{8}$$

where c_i is the modal density $\partial N/\partial\omega$ in room i. Thus the initial "leaking rate" σ_{21} from room 1 to 2 is $2\pi c_2\langle V^2\rangle$. Similarly, the initial leaking rate σ_{12} from room 2 to 1 following a deposition of energy in room 2 is $2\pi c_1\langle V^2\rangle$.

An expansion in powers of V is at best awkward for later times or larger V. While its secular terms may be accommodated by diagrammatic techniques and a proper definition of an irreducible vertex, the procedures are complicated. To date we have managed only to derive a set of classical diffusionlike equations (given below) [9], equations which show little sign of localization and/or are too difficult to solve. In [5], however, it was shown that the assumption of V small enough that each mode of one room is significantly coupled to, at most, one mode of the other allows Eqs. (7) to be solved and averaged in closed form. In this limit the mean energy in room 2 is given by

$$\langle E_2(t)\rangle = 2Ec_2\left\langle |V|\int_{-\infty}^{\infty} d\beta \frac{\sin^2(\sqrt{1+\beta^2}tV)}{1+\beta^2}\right\rangle, \tag{9}$$

showing that the energy in the second room is composed of a superposition of beat patterns. As $t\to\infty$ this approaches $E\, c_2\pi\langle|V|\rangle = E(\langle|V|\rangle/\langle V^2\rangle^{1/2})\,(\pi\sigma_{21}c_2/2)^{1/2}$. In the special case that V is a Gaussian random number, so that $(\langle|V|\rangle/\langle V^2\rangle^{1/2}) = \sqrt{2/\pi}$, we write that the late-time ratio of the energy in the source room 1 to the energy in the other room 2 is $\langle E_1(t=\infty)\rangle/\langle E_2(t=\infty)\rangle = 1/\sqrt{\sigma_{21}c_2}$. The ratio of the energy per mode is

$$\langle E_1(t=\infty)/c_1\rangle/\langle E_2(t=\infty)/c_2\rangle = (c_2/c_1)/\sqrt{\sigma_{21}c_2} = 1/\sqrt{\sigma_{12}c_1}. \tag{10}$$

Inasmuch as this is much greater than unity, we may term the system localized. The earlier work compared this asymptotic value and the dynamics predicted by Eq. (9) with that observed in direct numerical simulations and that observed in laboratory experiments on ultrasound in solid bodies. The essential features of the theory were confirmed.

The above theory fails to make predictions for stronger coupling or for systems composed of more than two substructures. In the following sections we introduce an *ad hoc* self-consistent hydrodynamical model for transport and localization among multiple substructures. We show that the new theory makes predictions in accord with the exact results above for weakly coupled pairs of substructures. We further show that in a continuum limit of many statistically identical well-coupled substructures in a chain, it resembles the Vollhardt-Wolfle [6] and van Tiggelen [7] self-consistent theories of transport dynamics. Finally, we compare its predictions with those of direct numerical simulations.

III. HYDRODYNAMICAL MODEL OF ENERGY FLOW AMONG SUBSTRUCTURES

Consider a system composed of several "rooms" α, each with spectral energy density e_α, and with energy flow rates $j_{\alpha\beta}$ from room β to α. Continuity states

$$\partial_t e_\alpha(t) = Q_\alpha(t) + \sum_\beta [j_{\alpha\beta}(t) - j_{\beta\alpha}(t)]. \tag{11}$$

In the frequency domain,

$$i\omega e_\alpha = Q_\alpha + \sum_\beta (j_{\alpha\beta} - j_{\beta\alpha}), \tag{12}$$

where ω is outer frequency, on a time scale of the energy flow. Q_α is the rate of deposit of spectral energy in room α.

Classical diffusion, or SEA, follows from invocation of a Fick-like constitutive relation

$$j_{\alpha\beta} = \kappa_{\alpha\beta}(e_\beta/c_\beta), \tag{13}$$

stating that energy flow from β to α is proportional to the energy per mode in room β [9]. κ is a dimensionless coupling, c_β is the modal density in room β, and $c = dN/d\omega$; it has units of time.

As an alternative to classical diffusion we suggest a current diminishing modification to Eq. (13), similar to the *ad hoc* hydrodynamical model of localization suggested by Vollhardt and Wolfle for continuous media [6,7]:

$$[i\omega + 1/\tau_{\alpha\beta}]j_{\alpha\beta} = i\omega\kappa_{\alpha\beta}(e_\beta/c_\beta). \tag{14}$$

We note in particular that $\tau=\infty$, or high frequency, corresponds to classical (SEA) diffusion. The phenomenological quantity τ may be taken to be a constant, as in [10], where that model was shown to incorrectly predict transport dynamics in multiply scattering continua or to be ω dependent as suggested below.

Continuity and the constitutive law may be combined to yield a governing equation for the energy density:

$$\sum_\beta [i\omega\delta_{\alpha\beta} - K_{\alpha\beta}(\omega)]e_\beta = Q_\alpha, \tag{15}$$

where

$$K_{\alpha\beta} \equiv \frac{\kappa_{\alpha\beta}/c_\beta}{1 + 1/i\omega\tau_{\alpha\beta}} - \delta_{\alpha\beta}\sum_\gamma \frac{\kappa_{\gamma\alpha}/c_\beta}{1 + 1/i\omega\tau_{\gamma\alpha}}. \tag{16}$$

The above governing equation has a fundamental solution P that satisfies

$$\sum_\beta [i\omega c_\beta\delta_{\alpha\beta} - K_{\alpha\beta}c_\beta]P_{\beta\nu} = \sum_\beta S_{\alpha\beta}P_{\beta\nu} = \delta_{\alpha\nu}; \quad P = S^{-1}. \tag{17}$$

$P_{\beta\nu}$ is the energy per mode in room β following an impulsive deposition of unit energy per frequency in room ν. In terms of P, e is given by

$$e_\beta = \sum_\nu P_{\beta\nu}Q_\nu c_\beta. \tag{18}$$

Reciprocity of wave fields implies reciprocity in P; thus, P must be symmetric [11]. This is turn implies that both κ and τ must be symmetric.

It is instructive to examine the hypothesis of a fixed τ and seek the corresponding behavior of P at early or late times. At early times—i.e., high ω—K and S reduce to their classical values and transport remains classically diffusive—i.e., in accord with SEA. At late times, low ω, S becomes

$$S_{\alpha\beta} = i\omega\left[c_\alpha\delta_{\alpha\beta} - \kappa_{\alpha\beta}\tau_{\alpha\beta} + \delta_{\alpha\beta}\sum_\gamma \kappa_{\gamma\alpha}\tau_{\gamma\alpha}\right] = i\omega Y_{\alpha\beta}. \tag{19}$$

$(Y^{-1})_{\alpha\beta}$ then describes the late-time steady-state distribution of energy per mode, E_α/c_α, in room α subsequent to a transient addition of unit energy in room β. Inasmuch as $(Y^{-1})_{\alpha\beta}$ is not independent of α, it violates equipartition and implies localization.

It remains to make a specification for the τ. We make the hypothesis

$$1/\tau_{\alpha\beta}(\omega) = i\omega P_{\alpha\beta}(\omega), \tag{20}$$

where τ is determined self-consistently from the dynamics P consequent to τ. The choice is motivated by its simplicity, its respect for the required symmetry $\tau_{\alpha\beta}=\tau_{\beta\alpha}$, and a notion that local diffusive properties must be renormalized, as in [6,7], by the local response of the entire structure. We show below that this leads to a predicted flow dynamics consistent with two special cases familiar from the literature, thus justifying Eq. (20) *a posteriori*.

A. Case 1, two rooms

Consider the case of two rooms of different sizes c_1 and c_2 coupled by $\kappa_{12}=\kappa$. There is one relaxation time $\tau=\tau_{12}$. We observe classical initial leaking rates (energy per time) flowing from room 1 to 2 after an addition of unit energy to room 1, $\sigma_{21}=\kappa/c_1$; similarly, $\sigma_{12}=\kappa/c_2$. On comparison with expression (8) derived in [5] and reviewed in the previous section, we therefore identify $\kappa=2\pi c_1c_2\langle|V|^2\rangle$.

P is the inverse of the 2×2 matrix with elements $S_{\alpha\beta}=[i\omega c_\beta\delta_{\alpha\beta}-K_{\alpha\beta}c_\beta]$:

$$S = \begin{bmatrix} i\omega c_1 + \kappa/(1 + 1/i\omega\tau) & -\kappa/(1 + 1/i\omega\tau) \\ -\kappa/(1 + 1/i\omega\tau) & i\omega c_2 + \kappa/(1 + 1/i\omega\tau) \end{bmatrix}, \tag{21}$$

$$P = S^{-1} = \frac{1}{i\omega[c_1c_2(i\omega + 1/\tau) + (\kappa c_1 + \kappa c_2)]} \times\begin{bmatrix} c_2(i\omega + 1/\tau) + \kappa & \kappa \\ \kappa & c_1(i\omega + 1/\tau) + \kappa \end{bmatrix}. \tag{22}$$

Our hypothesis (20) regarding τ then takes the form

$$\frac{1}{\tau(\omega)} = i\omega P_{21}(\omega) = \frac{\kappa}{[c_1c_2(i\omega + 1/\tau) + (\kappa c_1 + \kappa c_2)]}. \tag{23}$$

At weak coupling $\kappa\ll1$ and at low frequencies $\omega=0$; i.e., in the steady state, the above self-consistent equation for τ has a solution $\tau(0)=(c_1c_2/\kappa)^{1/2}$. In this same limit, the ratio of energy per mode in a source room 1 to that in the other room 2 is $P_{11}/P_{21}=[1+c_2/\kappa\tau(0)]\sim(c_2/\kappa c_1)^{1/2}=1/\sqrt{c_1\sigma_{12}}$. Localization is strong, of order $1/\sqrt{\kappa}$. That this agrees with the result (10) of the previous section is evidence in support of the hypothesis (20).

At strong coupling $\kappa\gg1$ and at low frequencies $\omega=0$—i.e., in the steady state—we recover $\tau=c_1+c_2$. This implies that the late time ratio P_{11}/P_{21} is $1+(c_2/\kappa)/(c_1+c_2)$. Localization is weak, of order $1/\kappa$.

B. Case 2, a one-dimensional continuum

Consider an infinite chain of rooms each of modal density c with nearest-neighbor couplings κ. All τ are identical. We observe initial leaking rates (energy per time flowing from a source room to an adjacent room after an addition of unit energy to source room) $\sigma=\kappa/c$. P is then the inverse of the infinite tridiagonal matrix $S_{\alpha\beta}=[i\omega c\,\delta_{\alpha\beta}-K_{\alpha\beta}c]$, $S_{nn}=i\omega c+2\kappa/(1+1/i\omega\tau)$; $S_{n,n+1}=S_{n+1,n}=-\kappa/(1+1/i\omega\tau)$.

P is given by

$$P_{nm} = \frac{1}{2\pi}\int_{-\pi}^{\pi} \frac{\exp\{iq(n-m)\}}{i\omega c + 2\kappa(1-\cos q)/(1+1/i\omega\tau)}dq. \tag{24}$$

Our hypothesis (20) regarding τ then takes the form

$$\frac{1}{\tau(\omega)} = i\omega P_{nn+1}(\omega) = \frac{1}{2\pi}\int_{-\pi}^{\pi} \frac{\exp\{-iq\}}{c + 2\kappa(1-\cos q)/(i\omega + 1/\tau)} dq. \tag{25}$$

We define a quantity $D(\omega)=(\kappa/c)/(1+1/i\omega\tau)$ and rewrite the above as

$$\frac{1}{\tau} = i\omega(\kappa/cD - 1) = \frac{1}{2\pi c}\int_{-\pi}^{\pi} \frac{\exp\{-iq\}}{1 + 2D(1-\cos q)/(i\omega)} dq \tag{26}$$

or, defining the classical diffusivity $D_0=\kappa/c$,

$$\frac{1}{D(\omega)} = \frac{1}{D_0} + \frac{1}{2\pi D_0 c}\int_{-\pi}^{\pi} \frac{\exp\{-iq\}}{i\omega + 2D(1-\cos q)} dq. \tag{27}$$

For $\omega \ll D_0$—i.e., for time scales longer than the short time required for classical diffusion between nearest-neighbor rooms—the integral is dominated by contributions from small q. The numerator becomes unity, and the denominator becomes the familiar diffusion pole $i\omega + Dq^2$. The above expression may then be recognized as similar to Vollhardt and Wolfle's self-consistent formula [6–8] for diffusivity $D(\omega)$ in a multiply scattering localizing continuum. The same conclusion follows for a two-dimensional array of rooms. In the continuum limit Eq. (27) differs from that of Vollhardt and Wolfle only in that the coefficient in front of the integral is too large by a factor of π. It is encouraging that Eq. (20) reduces to a familiar theory whose dynamics have been compared successfully to those of direct numerical simulations [8]. It is discouraging that the present prediction for one-dimensional (1D) localization length in terms of D_0 and c is less, by a factor of π, than that of [6,7]. It is also interesting that there is no special role played by backscatter P_{nn}, as in [6–8]. Instead, it is the scattering to nearest neighbors, $P_{n,n+1}$, which renormalizes the transport. In a continuum there is little distinction, but in a finite discrete structure, the difference can be significant.

The factor of π may be less serious than it appears. There is uncertainty over the precise value this coefficient should take [12]. Furthermore, it may be unreasonable to require a simple theory to correctly span the full range from two rooms to the continuum; the mechanisms responsible for localization in the two-room case [5] are different from those enhanced backscatter arguments invoked in the derivation of the Vollhardt-Wolfle theories for the continuum. Nevertheless, it is possible to construct alternatives to Eq. (20), designed to match known limits of weak coupling between two rooms and strong coupling in an infinite array of rooms. We could choose

$$1/\tau_{\alpha\beta}(\omega) = \frac{i\omega}{\pi} P_{\alpha\beta}(\omega)[1 + (\pi - 1)(i\omega)^2 c_\alpha c_\beta P_{\alpha\alpha} P_{\beta\beta}]. \tag{20'}$$

Inspection shows that, if P is highly diagonal, $\sim 1/i\omega c$, as it is in the two-room case with strong localization, then the second term is $\pi - 1$ and we recover Eq. (20). If the diagonal members of $i\omega cP$ are small, as they are in the infinite well-coupled array, the second term of Eq. (20′) is negligible and we recover Vollhardt and Wolfle. Analytically simpler than Eq. (20′), but arguably more *ad hoc*, is

$$1/\tau_{\alpha\beta}(\omega) = i\omega P_{\alpha\beta}(\omega) f(\kappa_{\alpha\beta}), \tag{20''}$$

where $f(\kappa)$ is a function that smoothly goes from unity to $1/\pi$ as κ goes from zero to infinity. There are surely many such generalizations of Eq. (20).

The hypothesis (20) and its kin have been given *primae facie* plausibility. It remains to examine more detailed implications and to compare them with direct numerical simulations. For the remainder of this work, we confine our attention to the simplest of the hypotheses (20) and leave alternatives to another occasion.

IV. DYNAMICS OF FLOW AMONG TWO OR THREE ROOMS

As an illustration of the present theory, we apply Eq. (20) to predict flow dynamics in two simple cases. Structures consisting of two or three statistically identical rooms in a uniform chain lead to relatively simple expressions. Furthermore, it becomes possible to compare predictions with the energy flows observed in straightforward direct numerical simulations.

A. Two rooms

Consider Eq. (23) in the case $c_1=c_2=c$:

$$\frac{1}{\tau(\omega)} = \frac{\kappa}{[c^2(i\omega + 1/\tau) + 2\kappa c]}. \tag{28}$$

Its solution is

$$\tau = c[1 + i\omega c/2\kappa + \sqrt{(1 + i\omega c/2\kappa)^2 + 1/\kappa}]. \tag{29}$$

Therefore,

$$P = \frac{1}{i\omega\kappa\tau}\begin{bmatrix} c(i\omega + 1/\tau) + \kappa & \kappa \\ \kappa & c(i\omega + 1/\tau) + \kappa \end{bmatrix}. \tag{30}$$

Taking time units such that $c=1$ and performing an inverse Fourier transform,

$$dP_{21}(t)/dt = \frac{1}{2\pi}\int_{-\infty}^{\infty} \frac{1}{\tau(\omega)} \exp\{i\omega t\} d\omega = \frac{1}{2\pi}\int_{-\infty}^{\infty} \frac{\exp\{i\omega t\}}{1 + i\omega/2\kappa + \sqrt{(1 + i\omega/2\kappa)^2 + 1/\kappa}} d\omega. \tag{31}$$

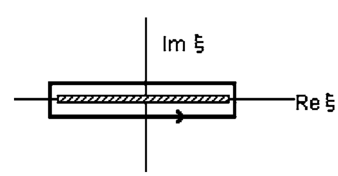

FIG. 1. Contour for the integral (32).

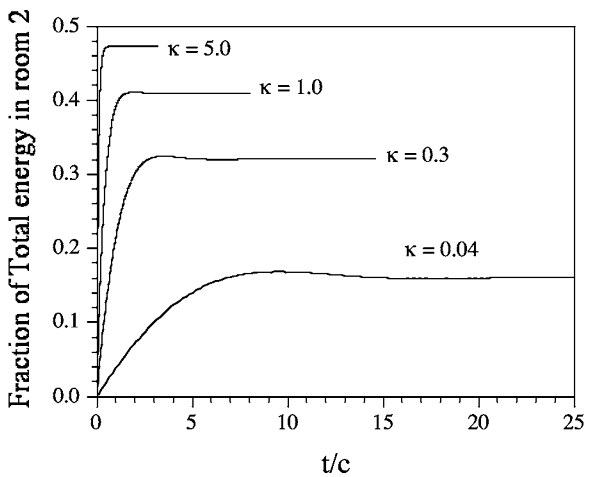

FIG. 2. Flow dynamics between two equal-sized rooms at various values of dimensionless coupling κ. Time is in units of modal density c.

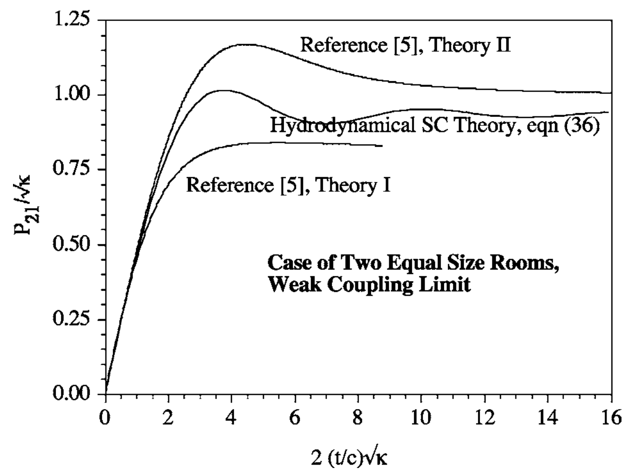

FIG. 3. Comparison of the theory of [5] with the hydrodynamical self-consistent theory (36). All curves are for the weak coupling limit $\kappa \ll 1$.

We change variables: $\omega = 2i\kappa + 2\xi\sqrt{\kappa}$, $d\omega = 2\sqrt{\kappa}d\xi$, and $1 + i\omega/2\kappa = i\xi/\sqrt{\kappa}$:

$$dP_{21}(t)/dt = \frac{\exp\{-2\kappa t\}}{i\pi}\kappa\int_{-\infty}^{\infty}\frac{\exp\{2i\xi\sqrt{\kappa t}\}}{\xi + \sqrt{\xi^2 - 1}}d\xi. \quad (32)$$

For $t > 0$, the integrand has branch points at $\xi = \pm 1$, with branch cut and deformed contour as indicated in Fig. 1.

We deform the integration contour so that it circles the branch cut and find

$$dP_{21}(t)/dt = \frac{\exp\{-2\kappa t\}}{i\pi}\kappa\int_{-1}^{1}\exp\{2i\xi\sqrt{\kappa t}\}\left[\frac{1}{\xi - i\sqrt{1-\xi^2}} - \frac{1}{\xi + i\sqrt{1-\xi^2}}\right]d\xi = \frac{\exp\{-2\kappa t\}}{i\pi}\kappa\int_{-1}^{1}[2i\sqrt{1-\xi^2}]\exp\{2i\xi\sqrt{\kappa t}\}d\xi. \quad (33)$$

We change variables once more, $\xi = \cos\phi$, and find

$$dP_{21}(t)/dt = 2\kappa\frac{\exp(-2\kappa t)}{\pi}\int_{0}^{\pi}[\sin^2\phi]\cos\{2\cos\phi\sqrt{\kappa t}\}d\phi, \quad (34)$$

which is found in the tables in [13]:

$$dP_{21}(t)/dt = \kappa\exp(-2\kappa t)\frac{J_1(2t\sqrt{\kappa})}{t\sqrt{\kappa}}. \quad (35)$$

This is plotted in Fig. 2 for various values of κ. The theory predicts flow over the full parameter range of dimensionless coupling κ and, in particular, correctly captures the overshoot phenomenon remarked upon elsewhere [5], in which the energy in room 2 rises to a level greater than its final steady state before relaxing to the steady state.

In the limit of very small κ, one may make comparisons with the dynamics predicted elsewhere [5]. In this case our P_{21} becomes

$$P_{21}(t) = \sqrt{\kappa}\int_{0}^{2t\sqrt{\kappa}}\frac{J_1(\zeta)}{\zeta}d\zeta. \quad (36)$$

This is plotted in Fig. 3, together with the predictions of [5]. The differences between the present theory and that of Ref. [5] are noteworthy. But they remain less than the variations within Ref. [5], between the case of assumed Gaussian statistics on the modal coupling strengths (theory II) or assumed product of two Gaussians (theory I).

B. Three rooms

For the case of three equal-sized rooms in a chain with uniform coupling κ, we again choose time units such that each room has $c=1$. P is the inverse of the 3×3 tridiagonal matrix $S = [i\omega\delta_{\alpha\beta} - K_{\alpha\beta}]$ $S_{11} = S_{33} = i\omega + \kappa/(1 + 1/i\omega\tau)$, $S_{12} = S_{21} = S_{23} = S_{32} = -\kappa/(1 + 1/i\omega\tau)$, $S_{22} = i\omega + 2\kappa/(1 + 1/i\omega\tau)$, and $S_{13} = S_{31} = 0$. P then is, where $X = \kappa/(1 + 1/i\omega\tau)$,

$$P = \frac{\begin{bmatrix}(i\omega+2X)(i\omega+X)-X^2 & X(i\omega+X) & X^2\\ X(i\omega+X) & (i\omega+X)^2 & X(i\omega+X)\\ X^2 & X(i\omega+X) & (i\omega+2X)(i\omega+X)-X^2\end{bmatrix}}{\{i\omega[i\omega+X][i\omega+3X]\}}. \quad (37)$$

Our hypothesis for τ then becomes

$$1/\tau = i\omega P_{21} = X/(i\omega + 3X) = \kappa/(3\kappa + i\omega + 1/\tau) \quad (38)$$

or

$$\tau = (3/2) + i\omega/2\kappa + \sqrt{(3/2 + i\omega/2\kappa)^2 + 1/\kappa}. \quad (39)$$

The expression for $P_{21}(t)$ is much as it was for the two-room case:

$$dP_{21}(t)/dt = \frac{1}{2\pi}\int_{-\infty}^{\infty} \frac{1}{\tau(\omega)} \exp\{i\omega t\} d\omega = \frac{1}{2\pi}\int_{-\infty}^{\infty} \frac{\exp\{i\omega t\}}{1.5 + i\omega/2\kappa + \sqrt{(1.5 + i\omega/2\kappa)^2 + 1/\kappa}} d\omega. \quad (40)$$

We change the variables $\omega = 3i\kappa + 2\xi\sqrt{\kappa}$, $d\omega = 2\sqrt{\kappa}d\xi$, and $1.5 + i\omega/2\kappa = i\xi/\sqrt{\kappa}$:

$$dP_{21}(t)/dt = \frac{\exp\{-3\kappa t\}}{i\pi}\kappa\int_{-\infty}^{\infty} \frac{\exp\{2i\xi\sqrt{\kappa}t\}}{\xi + \sqrt{\xi^2 - 1}} d\xi. \quad (41)$$

Further contour manipulations and variable changes are precisely as above, and we recover

$$dP_{21}(t)/dt = \kappa \exp\{-3\kappa t\}\frac{J_1(2t\sqrt{\kappa})}{t\sqrt{\kappa}}, \quad (42)$$

very similar to Eq. (35).

The calculation for P_{31} is slightly more complex:

$$dP_{31}(t)/dt = \frac{1}{2\pi}\int_{-\infty}^{\infty} \frac{X^2}{(i\omega + X)(i\omega + 3X)} \exp\{i\omega t\} d\omega = \frac{1}{2\pi}\int_{-\infty}^{\infty} \frac{\kappa^2 \exp\{i\omega t\}}{(i\omega + 1/\tau + \kappa)(i\omega + 1/\tau + 3\kappa)} d\omega. \quad (43)$$

The latter factor in the denominator is $\kappa\tau$ [cf. Eq. (38)]:

$$dP_{31}(t)/dt = \frac{\kappa}{2\pi}\int_{-\infty}^{\infty} \frac{\exp\{i\omega t\}}{[1 + (1.5 + i\omega/2\kappa + \sqrt{(1.5 + i\omega/2\kappa)^2 + 1/\kappa})\{i\omega + \kappa\}]} d\omega. \quad (44)$$

We again change variables $\omega = 3i\kappa + 2\zeta\sqrt{\kappa}$, $d\omega = 2\sqrt{\kappa}d\xi$, and $1.5 + i\omega/2\kappa = i\xi/\sqrt{\kappa}$:

$$dP_{31}(t)/dt = \frac{\kappa}{2\pi}\exp(-3\kappa t)\int_{-\infty-3i/\sqrt{\kappa}}^{\infty-3i/\sqrt{\kappa}} \frac{\exp\{2i\xi\sqrt{\kappa}t\}}{\{1 + [i\xi/\sqrt{\kappa} + \sqrt{-(\xi)^2/\kappa + 1/\kappa}](2i\xi\sqrt{\kappa} - 2\kappa)\}} 2\sqrt{\kappa}\, d\xi = \frac{\kappa}{2\pi}\exp(-3\kappa t)\int_{-\infty-3i/\sqrt{\kappa}}^{\infty-3i/\sqrt{\kappa}} \frac{\exp\{2i\xi\sqrt{\kappa}t\}}{[1 - (\xi + \sqrt{\xi^2 - 1})(2\xi + 2i\sqrt{\kappa})]} 2\sqrt{\kappa}\, d\xi. \quad (45)$$

The denominator has one root:

$$\xi^p = -i(4\kappa - 1)/(4\sqrt{\kappa}). \quad (46)$$

If $\mathrm{Im}(\xi^p)$ is negative ($\kappa > 1/4$), then this root is on the primary Riemann sheet. If positive ($\kappa < 1/4$), the pole migrates under the branch cut and does not appear on the primary sheet.

We deform the contour as before, so that it circles the branch cut. If $\kappa > 1/4$, the deformation also picks up the residue from the pole:

$$dP_{31}(t)/dt = X_{\mathrm{Br}} + X_{\mathrm{Po}} = \frac{\kappa^{3/2}}{\pi}\exp(-3\kappa t)\int_{-1}^{1}\left[\frac{\exp\{2i\xi\sqrt{\kappa}t\}}{[1 - (\xi - i\sqrt{1 - \xi^2})\{2\xi + 2i\sqrt{\kappa}\}]} - \frac{\exp\{2i\xi\sqrt{\kappa}t\}}{[1 - (\xi + i\sqrt{1 - \xi^2})\{2\xi + 2i\sqrt{\kappa}\}]}\right] d\xi + \frac{\kappa^{3/2}}{\pi}\exp(-3\kappa t) 2i\pi \frac{\exp\{2i\xi^p\sqrt{\kappa}t\}}{d[1 - (\xi + \sqrt{\xi^2 - 1})\{2\xi + 2i\sqrt{\kappa}\}]/d\xi|_{\xi^p}}\Theta(\kappa - 1/4). \quad (47)$$

On further manipulations, these quantities become

$$X_{\mathrm{Br}} = \frac{\kappa^{3/2}}{\pi}\exp(-3\kappa t)\int_{-\pi/2}^{\pi/2} \frac{-4i\cos^2\phi(\sin\phi + i\sqrt{\kappa})[1 - 4\kappa - 4i\sin\phi\sqrt{\kappa}]}{(1 - 4\kappa)^2 + 16\sin^2\phi\kappa} \exp\{2i\sin\phi\sqrt{\kappa}t\} d\phi \quad (48)$$

and

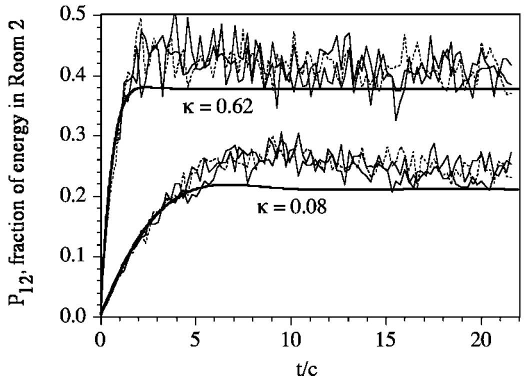

FIG. 4. For the case of two equal-sized rooms, the fraction of the total energy present in room No. 2 is plotted versus dimensionless time t/c. Smooth lines are the prediction of theory for the indicated values of κ. The jagged lines are the results of six distinct ensemble averages of direct numerical simulations.

$$X_{\mathrm{Po}} = -i\kappa^{3/2}\exp(-3\kappa t)\frac{\exp\{2i\xi^{p}\sqrt{\kappa t}\}}{[0.5/\sqrt{\xi^{p2}-1}+\xi^{p}+\sqrt{\xi^{p2}-1}]} \times\Theta(\kappa-1/4). \quad (49)$$

These expressions have been evaluated for two values of dimensionless coupling κ. They are plotted in Figs. 4 and 5.

V. DIRECT SIMULATIONS

Structures consisting of two or three rooms were studied by direct numerical simulations as well. The rooms were modeled by spatial and temporal finite differences with Dirichlet boundary conditions as described elsewhere [5,14]. Figure 6 illustrates one of these structures. Each room was of size 121×121 mesh spacings, with nominal wave speed c of unity. All four edges of each of the rooms were roughened, in the manner described elsewhere, with an average depth of that roughness equal to 3.5 mesh spacings. Thus the rooms were essentially of area $A=L^2=114\times114$. The rooms were coupled by clouds of 600 weak springs, as described in [5]. A single impulsive source was applied at the center of room No. 1 and the response monitored by eight receivers at random places in each room. The signal at each receiver was bandpass filtered at various frequencies of interest and squared, and the sum over the receivers in each room, the "energy" as a function of time, recorded.

This system has a Weyl-law modal density per room of

$$\partial N/\partial\omega = c = \omega A/2\pi c^2 - L/4c. \quad (50)$$

At the chief (inner) frequency of interest, $\omega=1.00$ at which wavelength is about 6 mesh spacings, this modal density c is 2040. An eigensolution of a small homogeneous (17×23) periodic boundary condition mesh shows that this estimate for modal density is too small, by about 6%, due to the anisotropy and dispersion of the spatial finite difference scheme. Thus we modify this estimate to $c=2160$.

The effective value of κ for these structures depends on the strength and number of the springs. Rather than attempt a theoretical relationship between κ and the spring stiffnesses, we opt instead to fit early time leaking rates dP_{12}/dt between two rooms to a value of κ. For 600 springs of stiffness 0.05, we observe at the frequency of interest $\omega=1.00$, a leaking rate (at times such that P_{12} remained linear in time, $P_{12}\sim\sigma t$, and averaged over 30 configurations) of $\sigma c=3.7\times10^{-5}$ per unit time, with an uncertainty of about 3%. This implies a dimensionless $\kappa=\sigma c=0.08$. A system with 600 springs of strength 0.15 was found to have a leaking rate (at this frequency ±5% and also averaged over 30 configurations) of $\sigma=0.000\,287$ and thus a dimensionless κ of 0.62.

In the following plots, the results from averaging the long-time response of the rooms over five configurations are presented. In Fig. 4 we present the case of two rooms, with 600 springs of stiffness 0.05 and 0.15, respectively. In Fig. 5, we show the case of three statistically equivalent rooms, coupled in a chain by sets of 600 springs of the same stiffnesses. The appropriate predictions of the previous section are plotted on the same scales by identifying the value of the

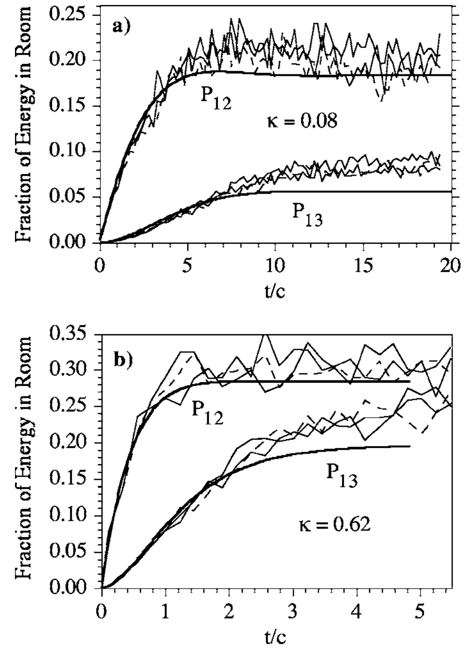

FIG. 5. For the case of three equal-sized rooms, the fraction of the total energy present in rooms Nos. 2 and 3 is plotted versus dimensionless time t/c. Smooth lines are the prediction of theory for the indicated values of κ. The jagged lines are the result of three distinct ensemble averages of direct numerical simulations. (a) For springs of stiffness 0.05, (b) for a more strongly coupled system with springs of stiffness 0.15.

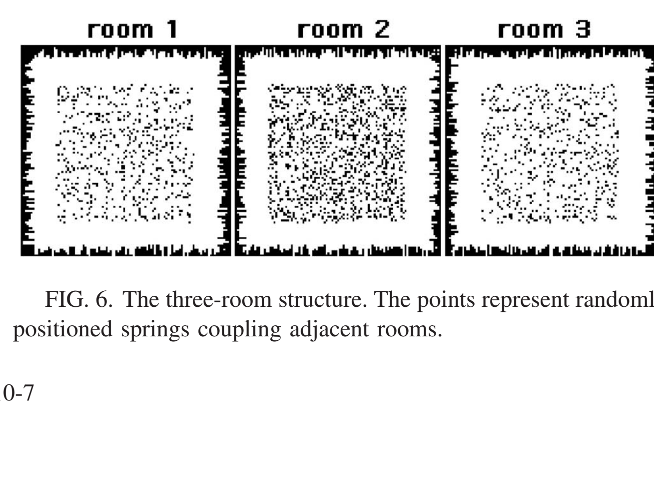

FIG. 6. The three-room structure. The points represent randomly positioned springs coupling adjacent rooms.

coupling strength κ, as discussed immediately above, while recognizing the ratio of time scales (a factor of $c=2160$).

The agreement is not perfect, and indeed the disagreements appear to be statistically significant. The behaviors under three different random number seeds are essentially the same. It is possible that the disagreements at late times could be ameliorated by slightly greater guesses for the dimensionless couplings κ, at the cost of generating theoretical curves with greater initial slope and less agreement at early times. Alternatively, one could maintain the agreement at early times, where theory is well established, while improving agreement at later times, by choosing greater values for both c and κ. (The early time slope is κ/c.) But the c's value is not subject to much uncertainty, and the changes would have to be large; no plausible adjustment of our estimates for κ and c could bring the predictions for P_{13} into agreement with the numerical simulations. The disagreements could also be ascribed to an as-yet-unascertained mechanism that generates an extra factor of $1/\pi$ at longer ranges, perhaps a theory like [Eq. (20′) or (20″)]. It may be that the difference in P_{13} is the sign, in a three-room structure, of the failure to reduce to the Vollhardt-Wolfle model for an infinite chain. The sense of the differences seen in the three-room case in Fig. 5(a) is consistent with the sense of the missing factor of π in Eq. (27). While the agreement is imperfect, the imperfection must be judged against the simplicity of the theory (20) and its independence from any parameters other than those (κ, c) required by classical theories. It may also be judged in context: the absence of any other theories.

VI. SUMMARY

A self-consistent theory has been hypothesized for transport and localization among coupled substructures. It reduces to conventional statistical energy analysis in the strong-coupling limit and predicts localization in the limit of weak coupling. It is parameter free in the sense that it calls only for modal densities in each substructure and for coupling strengths between them, the same parameters required by classical theories. In the limit of two weakly coupled substructures, with random modal coupling strengths having a Gaussian distribution, it agrees with an exact prediction for the degree of localization, but disagrees slightly with the exact dynamics. In the limit that the structure becomes a well-coupled continuum, it reduces, within a factor of π, to the Vollhardt-Wolfle self-consistent theory for transport and localization in multiply scattering continua. The theory imperfectly matches to that theory and to our direct numerical simulations. At this point one cannot apply this model with any confidence to more general structures. Improved theories are needed.

A diagrammatic derivation of an equation like Eq. (20) that is analogous to that of Vollhardt and Wolfle [6] or a supersymmetry calculation along the lines of [15] is to be desired.

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