A random matrix model for the non-perturbative response of a complex quantum system

# A random matrix model for the non-perturbative response of a complex quantum system

Michael Wilkinson† and Elizabeth J Austin†

Laboratoire de Physique Quantique, Université Paul Sabatier, 118, Route de Narbonne, F-31062, Toulouse Cédex, France

**Abstract.** We consider the dynamics of a complex quantum system subjected to a time-dependent perturbation, using a random matrix approach. The dynamics are described by a diffusion constant characterizing the spread of the probability distribution for the energy of a particle which was initially in an eigenstate.

We discuss a system of stochastic differential equations which are a model for the Schrödinger equation written in an adiabatic basis. We examine the dependence of the diffusion constant $D$ on the rate of change of the perturbation parameter, $\dot{X}$. Our analysis indicates that $D \propto \dot{X}^2$, in agreement with the Kubo formula, up to a critical velocity $\dot{X}^*$; for faster perturbations, the rate of diffusion is lower than that predicted from the Kubo formula. These predictions are confirmed in numerical experiments on a banded random matrix model. The implications of this result are discussed.

## 1. Introduction

The objective of the work described in this paper was to understand the response of complicated quantum systems to a time-dependent variation of the Hamiltonian. We concentrate on analysing a regime in which the conditions for quantum mechanical perturbation theory are not applicable. This is a problem of considerable importance, because the conditions for perturbation theory require that some measure of the strength of the perturbation should be small compared with the typical separation of energy levels. In solid state physics, we are usually concerned with bulk properties, and the separation of individual energy levels is infinitesimal. It is therefore very important to analyse the problem of perturbations which are large from the point of view of quantum perturbation theory.

Complex systems without symmetries or constants of motion are expected to have some universal statistical properties which can be modelled by suitably defined random matrix ensembles [1]. Random matrix methods have been used successfully to model statistical properties of the spectra of nuclei [1], where the complexity arises because there are many degrees of freedom, and systems with few degrees of freedom in which there is chaotic classical motion [2]. We will consider the dynamics of a random matrix model for a complex quantum system with a time-dependent Hamiltonian. This extends earlier work [3], in which we modelled the response to a low-frequency perturbation, using a parameter-dependent version of the standard Gaussian random matrix ensembles. In the

† Permanent Address: Department of Physics and Applied Physics, John Anderson Building, University of Strathclyde, Glasgow G4 0NG, UK.

present paper we consider a more general model which introduces a surprising new feature, not present in the dynamics of the parametrized Gaussian ensembles.

The response of systems to a large time-dependent perturbation can usually be characterized by a diffusion constant $D$ [4]. We expand the wavefunction in an adiabatic basis:

$$|\psi(t)\rangle = \sum_n a_n(t) \exp[-i\theta_n(t)] \, |\phi_n(t)\rangle \tag{1.1}$$

where $|\phi_n(t)\rangle$ are eigenstates of the instantaneous Hamiltonian, and the phases $\theta_n$ will be discussed in section 2. It is typically found that the second moment of the probability distribution resulting from a single eigenstate (the $n$th, say) at $t = 0$ has a diffusive growth:

$$\Delta(t) = \sum_m |a_m(t)|^2 (n - m)^2 \sim 2Dt. \tag{1.2}$$

This growth may, in some systems, be limited by the finite number of states available, or by an Anderson localization effect [5, 3], and the diffusion constant may vary as a function of energy. We will assume that the response of the system is a diffusive spread of the wavepacket described by (1.2) (possibly preceded by a brief transient), and the dynamics of the system will be characterized by calculating the diffusion constant $D$.

Low lying states of many electron systems are usually modelled by a system of independent fermions. The diffusion constant $D$ is proportional to the rate of dissipation in such a system [6, 4]:

$$\left\langle \frac{dE_T}{dt} \right\rangle = D/\rho \tag{1.3}$$

where $E_T$ is the total energy of the electrons, and $\rho$ is the single-particle density of states. Usually, the rate of dissipation is calculated using the Kubo formula [7] (the version which is most directly applicable to our work appears in a later paper by Greenwood [8]). We will be largely concerned with the comparison between this approach and our results. The Kubo formula predicts that, if the perturbation parameter varies sinusoidally,

$$X(t) = X_0 \sin \omega t \tag{1.4}$$

the rate of dissipation (for a system initially in the ground state with all states above the Fermi energy $E_F$ empty) is

$$\left\langle \frac{dE_T}{dt} \right\rangle = \tfrac{1}{2} \Sigma(\omega) X_0^2 \omega^2. \tag{1.5}$$

Here the constant $\Sigma(\omega)$ is given by

$$\Sigma(\omega) = \pi \hbar \rho^2 \sigma^2(E_F, \hbar\omega) \tag{1.6}$$

where $\sigma^2(E, \Delta E)$ is the mean-squared matrix element of the perturbation, for pairs of states with mean energy $E$ and energy difference $\Delta E$ (the quantity $\sigma^2$ will be defined more precisely in section 3). The coordinate $X$ might represent a magnetic flux threaded through a loop, in which case $\Sigma(\omega)$ is the frequency dependent electrical conductance at zero temperature. If the rate of change of the perturbation parameter is small, we might

expect that the rate of dissipation is a function of the instantaneous velocity, $\dot{X} = dX/dt$. For consistency with the Kubo formula, the rate of dissipation must be

$$\left\langle \frac{dE_T}{dt} \right\rangle = \Sigma(0)\dot{X}^2. \tag{1.7}$$

The mean-square matrix element $\sigma^2(E, \Delta E)$ is expected to become very small for energy differences larger than some characteristic value $\Delta E_0$. It would therefore be expected that the conductance $\Sigma(\omega)$ would decrease for frequencies above $\omega^* \sim \Delta E_0/\hbar$, and this conclusion is correct in the perturbative regime. In this paper we will show that (at least for one random matrix model), in the non-perturbative regime the response to a periodic perturbation is reduced above a critical value of the *velocity*, $\dot{X} = X_0\omega$, rather than a critical frequency.

This conclusion will be motivated by considering a stochastic differential equation, which is a reasonable model for the adiabatic representation of the Schrödinger equation in the non-perturbative regime. In section 2 we introduce the adiabatic form of the Schrödinger equation, and discuss the extent to which its evolution is reversible under reversal of the change of the perturbation parameter. Section 3 discusses the definition of the matrix element variance $\sigma^2(E, \Delta E)$, and considers the various dimensionless parameters which determine the response of the system, including a dimensionless measure of the velocity, $\eta \propto \dot{X}$. In section 4 we introduce a system of stochastic differential equations which models the behaviour of the Schrödinger equation in the limit of large perturbations, and present a heuristic theory for the diffusion constant $D$ of this system. Our formula for the diffusion constant $D(\dot{X})$ is applied to the Schrödinger equation in section 5. We find, remarkably, that this model reproduces the Kubo formula exactly when $\eta \ll 1$, despite the very different form of the theory. We also predict a non-perturbative regime which has not previously been characterized, in which the diffusion constant is smaller than that predicted by the Kubo formula when $\eta \gg 1$.

This prediction is tested numerically in section 6. We describe numerical results for the time-dependent Schrödinger equation for a banded random matrix model, which are strong evidence that this regime exists. Sections 7 and 8 discuss the implications for physical problems, including a model for electrical conduction. Our results show that the response of at least one system is at variance with the Kubo formula in a physically significant non-perturbative regime, and that the use of the Kubo formula approach as a quantum theory for electrical conductance needs to be re-assessed. We mention that the applicability of the Kubo formula to systems subjected to realistically sized perturbations has also been questioned by van Kampen [9].

## 2. Equations of motion and their irreversibility

In this section we discuss the adiabatic form of the Schrödinger equation and its advantages for examining the response of a system to large perturbations. We also discuss the circumstances under which the motion is reversible under reversing the time dependence of the parameter $X(t)$.

We consider a system with a Hamiltonian $\hat{H}$ depending on a parameter $X$. The parameter is time-dependent, and the rate of change of $X(t)$ is $\dot{X}$. The solution $|\psi(t)\rangle$ of the Schrödinger equation will be expanded in the adiabatic basis, as in (1.1), where the

states $|\phi_n(t)\rangle$ are eigenfunctions of the instantaneous Hamiltonian $\hat{H}(X(t))$, and the $\theta_n(t)$ are integrals of the instantaneous eigenvalues $E_n(t)$

$$\theta_n(t) = \frac{1}{\hbar} \int_0^t \mathrm{d}t' \, E_n(t') \,. \tag{2.1}$$

It will be asssumed that the phases of the eigenfunctions are chosen so as to satisfy the standard connection rule for adiabatic problems [10]:

$$\left\langle \phi_n \left| \frac{\partial \phi_n}{\partial X} \right. \right\rangle = 0 \,. \tag{2.2}$$

Substituting (1.1) into the time-dependent Schrödinger equation and making use of (2.1) and (2.2), the equation of motion of the expansion coefficients $a_n(t)$ is

$$\dot{a}_n = \dot{X} \sum_{m \neq n} \frac{\langle \phi_n | \frac{\partial \hat{H}}{\partial X} | \phi_m \rangle}{E_m - E_n} \exp[\mathrm{i}(\theta_n - \theta_m)] \, a_m \tag{2.3}$$

which we will refer to as the adiabatic representation of the Schrödinger equation. Note that both the energies $E_n$ and the matrix elements $\langle \phi_n | \partial \hat{H}/\partial X | \phi_m \rangle$ in these equations of motion depend on the parameter $X(t)$. Their equations of motion are discussed by Pechukas [11].

An inconvenient feature of the adiabatic representation is that the coefficients $c_n(t)$ representing a constant state vector are time-dependent. If

$$|\Phi\rangle = \sum_n c_n(t) \, |\phi_n(t)\rangle \tag{2.4}$$

is a time-independent state vector, it is easy to show (by applying first order perturbation theory to the basis states $|\phi_n(X)\rangle$) that the coefficients $c_n(t)$ satisfy the equations of motion

$$\dot{c}_n = \dot{X} \sum_{m \neq n} \frac{\langle \phi_n | \frac{\partial \hat{H}}{\partial X} | \phi_m \rangle}{E_m - E_n} \, c_m \tag{2.5}$$

which are the same as (2.3) with the phase factor removed. It is therefore important to distinguish between the real dynamics and the time dependence of a fixed state vector given by (2.5). Our justification for using the adiabatic basis is that it is more convenient for looking at large perturbations because the equations of motion contain $\dot{X}$ rather than the large parameter $X$.

It is also necessary to consider the extent to which the evolution generated by (2.3) is reversible if the path $X(t)$ is reversed. Consider what happens if $X$ is taken from $X_i$ to $X_f$ between $t = 0$ and $t = T$ with time dependence $X = F(t)$, and then the path is reversed so that $X$ returns to $X_i$ at time $t = 2T$, with time dependence $X(t) = F(2T - t)$. The evolution generated by (2.3) can be represented by a unitary matrix $\hat{U} = \{U_{nm}\}$:

$$a_n(t_f) = \sum_m U_{nm}(t_f, t_i) \, a_m(t_i) \qquad \hat{U}^{-1} = \hat{U}^{T*} \tag{2.6}$$

and by changing the sign of $\mathrm{d}t$ in (2.3) it is clear that the evolution operator for the reversed path satisfies

$$\hat{U}(2T, T) = \hat{U}^{-1*}(T, 0) = \hat{U}^T(T, 0) \,. \tag{2.7}$$

This should be compared with the evolution of the coefficients of a fixed state vector, given by (2.5). In this case the transformation depends only on the value of $X$, and not upon the history of $X(t)$, and it is orthogonal because the equation of motion is real:

$$c_n(X_f) = \sum_m O_{nm}(X_f, X_i) \, c_m(X_i) \qquad \hat{O}^{-1} = \hat{O}^T \tag{2.8}$$

and

$$\hat{O}(X_i, X_f) = \hat{O}^T(X_f, X_i) = \hat{O}^{-1}(X_f, X_i) \tag{2.9}$$

so that the evolution of the coefficients of a fixed state is exactly reversible. Clearly, if the imaginary parts of the unitary matrix $\hat{U}(T, 0)$ are small, the product

$$\hat{U}(2T, 0) = \hat{U}(2T, T) \, \hat{U}(T, 0) = \hat{U}^T(T, 0) \, \hat{U}(T, 0) \tag{2.10}$$

will be close to the identity, and the motion will be reversible. If the imaginary parts of the elements of $\hat{U}(T, 0)$ are comparable to the real parts, there is no reason to expect that reversing the path $X(t)$ will cause a reversal of the motion.

## 3. Dimensionless parameters characterizing the dynamics

In order to analyse the equations of motion (2.3), we need to specify some information about the energies $E_n(t)$ and the matrix elements $(\partial H/\partial X)_{nm}(t) = \langle \phi_n | \partial \hat{H}/\partial X | \phi_m \rangle$. The energy levels are usefully characterized by the smoothed density of states

$$\rho(E) = \sum_n \delta_\epsilon(E - E_n) \tag{3.1}$$

where $\delta_\epsilon(x)$ is a 'smoothed delta function', i.e. a function which has negligible weight outside an interval of width $O(\epsilon)$ centred on 0, and for which the integrated weight is unity (an example would be the Gaussian function $\exp(-x^2/2\epsilon^2)/\sqrt{2\pi}\epsilon$). The averaging interval $\epsilon$ should be large compared to the typical separation of energy levels, and small compared to other energy scales; there are a wide variety of systems for which this separation of scales exists, including bulk systems such as solids, and semiclassical systems.

The off-diagonal matrix elements are usually Gaussian distributed with mean value zero [12], and with a variance $\sigma^2$ which is a function of the mean energy $E = \frac{1}{2}(E_n + E_m)$ and the energy difference $\Delta E = E_n - E_m$; by analogy with (3.1), we define

$$\sigma^2(E, \Delta E) = \frac{1}{\rho^2(E)} \sum_n \sum_{m \neq n} \left| \left( \frac{\partial H}{\partial X} \right)_{nm} \right|^2 \delta_\epsilon\big(E - \tfrac{1}{2}(E_n + E_m)\big) \, \delta_\epsilon(\Delta E - (E_n - E_m)) . \tag{3.2}$$

If the system has a classical limit, both $\rho(E)$ and $\sigma^2(E, \Delta E)$ can be calculated in terms of classical quantities in the limit $\hbar \to 0$: see [2, 13], respectively.

The time dependence of $X(t)$ may be characterized by a rate of change $\dot{X}$, and (unless $X(t)$ is unbounded) by an amplitude $X_0$. We will consider two specific cases, in which $X(t)$ is linear, $X(t) = \dot{X}t$, or sinusoidal, $X(t) = X_0 \sin(\omega t)$. In the latter case $\dot{X}$ will be taken to be the RMS velocity, $\dot{X} = X_0 \omega/\sqrt{2}$.

We will assume, for simplicity, that the variation of $\rho(E)$ and $\sigma^2(E, \Delta E)$ with $E$ does not play a rôle in the model, and that the only important energy scale in $\sigma^2(E, \Delta E)$ concerns the variation with $\Delta E$. We will characterize this energy scale by the parameter $\Delta E_0$, defined by

$$\Delta E_0 = \frac{1}{\sigma^2(E_F, 0)} \int_0^\infty d\Delta E \, \sigma^2(E_F, \Delta E). \tag{3.3}$$

We will refer to $\Delta E_0$ as the 'support' of the function $\sigma^2(E, \Delta E)$ in the variable $\Delta E$, and define the support of other functions in the same manner. For a function $f(x)$ which decays rapidly as $x \to \pm\infty$ this definition gives an indication of the size of the interval over which the function is significantly different from zero; this is of course not the same as the mathematical definition of the support. In the case of systems with a classical limit, the characteristic scale of variations of $\rho$ and $\sigma^2$ with $E$ is independent of $\hbar$, whereas the support of $\sigma^2$ in $\Delta E$ is O($\hbar$) [13]: this justifies the assumption of the separation of energy scales referred to above. Also, $\rho \sim \hbar^{-d}$, where $d$ is the number of degrees of freedom, so that (for $d > 1$) the typical separation of energy levels is small compared to $\Delta E$. This means that there is no difficulty in choosing a values for $\epsilon$ in (3.1) and (3.2) which are large compared to the level spacing, but small compared to other relevant energy scales.

The quantities entering into the equation of motion will therefore be characterized by the parameters

$$\rho \quad \sigma_0^2 = \sigma^2(E_F, 0) \quad \Delta E_0 \quad X_0 \quad \dot{X} \quad \hbar. \tag{3.4}$$

From these we can form three independent dimensionless combinations:

$$\kappa = \rho^2 \sigma_0 \hbar \dot{X} \qquad \eta = \rho \sigma_0 \hbar \dot{X} / \Delta E_0 \qquad \chi = \rho \sigma_0 X_0. \tag{3.5}$$

These parameters can be understood as follows. Perturbation theory shows that the timescale upon which the matrix elements $\langle \phi_n | \partial \hat{H} / \partial X | \phi_m \rangle$ decorrelate is $\tau_c \sim (\rho \sigma_0 \dot{X})^{-1}$, which gives rise to an energy scale $\hbar / \tau_c = \hbar \rho \sigma_0 \dot{X}$. The first two dimensionless parameters are obtained by dividing this energy scale by $\rho^{-1}$ and $\Delta E_0$, respectively. Because we assume that $\Delta E_0 \rho \gg 1$, we have $\kappa \gg \eta$. The third parameter $\chi$ is a dimensionless measure of the strength of the perturbation. Our earlier paper [3] considered a system in which $\sigma^2$ was independent of $\Delta E$, so that the parameter $\eta$ was always zero. The interpretation of the parameter $\kappa$ was discussed in [4, 6]: when $\kappa$ is small and $\chi \gg 1$, Landau–Zener transitions are the dominant mechanism for excitation of the system.

## 4. A stochastic model for the Schrödinger equation

In order to solve (2.3) in the non-perturbative regime, we must have information about the variation of the the energy levels and matrix elements as a function of the parameter $X$. The energy levels and matrix elements satisfy a system of coupled nonlinear differential equations [11]. It is known that these equations are at least partially integrable, but the constants of motion are in the form of constraints involving all the energy levels and matrix elements [14]. We will simplify this complex problem by regarding the matrix elements as independent Gaussian random variables, with a given autocorrelation function. The matrix

elements will be assumed to have a correlation function $C(t)$, such that (for $n \geqslant m$ and $n' \geqslant m'$)

$$\left\langle \left(\frac{\partial H}{\partial X}\right)_{nm}(t) \left(\frac{\partial H}{\partial X}\right)^*_{n'm'}(t')\right\rangle = \delta_{nn'} \delta_{mm'} \sigma^2(\bar{E}, \Delta E) C(t - t') \tag{4.1}$$

where $\bar{E} = \frac{1}{2}(E_n + E_m)$ and $\Delta E = E_n - E_m$. It is clear from perturbation theory that the characteristic timescale for the decay of correlations of the matrix elements is $\tau_c = (\sigma_0 \rho \dot{X})^{-1}$. The assumption that the matrix elements are uncorrelated is an oversimplification, and we will consider a refinement of this picture in a later paper.

Even with this simplifying assumption, (2.3) is very hard to solve directly. We will therefore consider a further simplification of the model, in which (2.3) is replaced by a system of differential equations of the form

$$\dot{a}_n(t) = \epsilon \sum_{m \neq n} Z_{nm}(t) \exp[i\lambda(n - m)t] a_m(t) \tag{4.2}$$

where the $Z_{nm}(t)$ are elements of an anti-Hermitean matrix ($Z_{nm} = -Z^*_{mn}$, $Z_{nn} = 0$). The coefficients $Z_{nm}(t)$ are complex random variables, with real and imaginary parts independently Gaussian distributed, and with correlation function

$$\langle Z_{nm}(t_1) Z^*_{n'm'}(t_2)\rangle = \delta_{nn'} \delta_{mm'} f(n - m) C(t_1 - t_2) \qquad C(0) = 1. \tag{4.3}$$

This is a reasonable model for equation (2.3) if we make the identifications $\epsilon = \dot{X}$, $\lambda = (\hbar\rho)^{-1}$, and $f(\Delta n) = \sigma^2(\Delta E)/\Delta E^2$ (where $\Delta E = \Delta n/\rho$).

It is useful to consider rescaling (4.2) into a dimensionless form, in which the correlation time is $\tau_c = O(1)$ and the function $f(n)$ is chosen such that $f(1) = O(1)$: making the transformations $t \to t' = \rho\sigma_0 \dot{X} t$ and $Z_{nm} \to Z'_{nm} = Z_{nm}/\rho\sigma_0$, gives an equation of the same form as (4.2) in which we have

$$f(1) = O(1) \qquad \tau_c = O(1) \qquad \epsilon = O(1) \qquad \lambda = O(\kappa^{-1}) \tag{4.4}$$

where $\kappa = \rho^2 \sigma_0 \hbar \dot{X}$. First we consider the solution of the dimensionless form of (4.2) in the perturbative case where $\epsilon$ is small; later we make a hypothesis about how the expression should be modified in the intermediate coupling regime (i.e. $\epsilon = O(1)$), which models the adiabatic Schrödinger equation.

Formally, the solution of (4.2) is

$$a_n(t) = \sum_m U_{nm}(t, 0) a_m(0) \tag{4.5}$$

where the matrix elements of the evolution operator $\hat{U} = \{U_{nm}\}$ satisfy a 'Dyson equation' of the form

$$U_{nm}(t, 0) = \delta_{nm} + \epsilon \sum_k \int_0^t \mathrm{d}t' Z_{nk}(t') U_{km}(t', 0) \exp[i\lambda(n - k)t']. \tag{4.6}$$

A perturbation expansion of $\hat{U}(t, 0)$ can be obtained by iterating (4.6).

Substituting (4.6) into (4.5), and taking the modulus squared, we obtain the following exact equation:

$$|a_n(t)|^2 - |a_n(0)|^2 = 2\,\mathrm{Re}\,\epsilon \sum_m \int_0^t \mathrm{d}t'\, Z_{nm}(t')\, \exp[\mathrm{i}\lambda(n-m)t']\, a_n^*(0)\, a_m(0)$$

$$+ 2\,\mathrm{Re}\,\epsilon^2 \sum_m \sum_{m'} \int_0^t \mathrm{d}t_1 \int_0^{t_1} \mathrm{d}t_2\, Z_{nm}(t_1)\, Z_{mm'}(t_2)$$

$$\times \exp[\mathrm{i}\lambda\{(n-m)t_1 + (m-m')t_2\}]\, a_n^*(0)\, a_{m'}(t_2)$$

$$+ \epsilon^2 \sum_m \sum_{m'} \int_0^t \mathrm{d}t_1 \int_0^t \mathrm{d}t_2\, Z_{nm}^*(t_1)\, Z_{nm'}(t_2)$$

$$\times \exp[\mathrm{i}\lambda\{(n-m')t_2 - (n-m)t_1\}]\, a_m^*(t_1)\, a_{m'}(t_2). \tag{4.7}$$

We now consider a perturbative solution of (4.7), which is valid in the limit $\epsilon \to 0$. We will assume that $t \gg \tau_c$, but that $t$ is small enough that, on the right hand side of (4.7) we can approximate the amplitudes $a_n(t)$ by their values at $t = 0$; these assumptions are clearly consistent if $\epsilon$ is sufficiently small. If the initial amplitudes $a_n(0)$ have randomly chosen phases, so that $\langle a_n(0) \rangle = 0$, then in the RHS of (4.7) we will put

$$\langle a_n(t_1) a_m^*(t_2) \rangle \sim \delta_{nm} P_m(0) \tag{4.8}$$

where $P_n(t) = \langle |a_n(t)|^2 \rangle$ is the average probability of occupation of the $n$th level at time $t$. Using (4.8), the average of (4.7) is therefore

$$P_n(t) - P_n(0) = \langle |a_n(t)|^2 \rangle - |a_n(0)|^2$$

$$\sim 2\,\mathrm{Re}\,\epsilon^2 \sum_m \int_0^t \mathrm{d}t_1 \int_0^{t_1} \mathrm{d}t_2\, \langle Z_{nm}(t_1) Z_{mn}(t_2) \rangle\, \exp[\mathrm{i}\lambda(n-m)(t_1-t_2)]\, P_n(0)$$

$$+ \epsilon^2 \sum_m \int_0^t \mathrm{d}t_1 \int_0^t \mathrm{d}t_2\, \langle Z_{nm}^*(t_1) Z_{nm}(t_2) \rangle\, \exp[\mathrm{i}\lambda(n-m)(t_2-t_1)]\, P_m(0).$$

$$\tag{4.9}$$

Now because the time $t$ is assumed to be large compared to the correlation time $\tau_c$, the double integrals can be approximated as follows:

$$P_n(t) \sim P_n(0) + \epsilon^2 t \sum_m \int_{-\infty}^\infty \mathrm{d}\tau\, \langle Z_{nm}(\tau) Z_{nm}^*(0) \rangle\, \exp[\mathrm{i}\lambda(n-m)\tau]\, (P_m(0) - P_n(0))$$

$$\tag{4.10}$$

(equation (4.3) was used in simplifying this result). Differentiation of (4.10) shows that the occupation probabilities satisfy the equation of motion

$$\frac{\mathrm{d}P_n}{\mathrm{d}t} = \sum_m R_{nm}\, (P_m - P_n) \tag{4.11}$$

where the rate constants $R_{nm}$ are given by

$$R_{nm} = \epsilon^2 \int_{-\infty}^\infty \mathrm{d}\tau\, \langle Z_{nm}(\tau) Z_{nm}^*(0) \rangle\, \exp[\mathrm{i}\lambda(n-m)\tau]$$

$$= \epsilon^2 f(n-m) \int_{-\infty}^\infty \mathrm{d}\tau\, C(\tau)\, \exp[\mathrm{i}\lambda(n-m)\tau]. \tag{4.12}$$

If the averaged occupation probability is a slowly varying function of $n$, the difference $P_m - P_n$ in (4.11) can be Taylor expanded in $\Delta n = m - n$

$$P_m = P_n + \frac{\partial P}{\partial n} \Delta n + \frac{1}{2} \frac{\partial^2 P}{\partial n^2} \Delta n^2 + O(\Delta n^3) \tag{4.13}$$

and the equation of motion (4.11) can be approximated by a diffusion equation

$$\frac{\partial P}{\partial t} = D \frac{\partial^2 P}{\partial n^2} \tag{4.14}$$

with diffusion constant

$$D = \tfrac{1}{2} \sum_m R_{nm} (n - m)^2 . \tag{4.15}$$

The arguments leading to (4.4) indicate that our primary interest is in the case where $\epsilon = O(1)$. In the case where $\epsilon$ is not small, we will assume that the dynamics can be approximated by a rate equation of the form (4.11), and that the rate constants $R_{nm}$ can be estimated from the following argument. The ensemble average of the final summation of (4.7), representing transitions into the $n$th level from all the other states, is approximated as follows:

$$\epsilon^2 \sum_m \sum_{m'} \int_0^t dt_1 \int_0^t dt_2 \langle Z_{nm}^*(t_1) Z_{nm'}(t_2) a_m^*(t_1) a_{m'}(t_2) \rangle \exp[i\lambda \{(n - m')t_2 - (n - m)t_1\}]$$

$$\sim \epsilon^2 \sum_m \sum_{m'} \sum_k \int_0^t dt_1 \int_0^t dt_2 \langle Z_{nm}^*(t_1) Z_{nm'}(t_2) U_{mk}^*(t_1, t_2) \rangle$$

$$\times \langle a_k^*(t_2) a_{m'}(t_2) \rangle \exp[i\lambda(n - m')t_1 - (n - m)t_2]$$

$$\sim \epsilon^2 \sum_m \int_0^t dt_1 \int_0^t dt_2 \langle Z_{nm}^*(t_1) Z_{nm}(t_2) \rangle \langle U_{mm}^*(t_1, t_2) \rangle$$

$$\times \exp[i\lambda(n - m)(t_1 - t_2)] P_m(t_2) \sim \int_0^t dt' \sum_m R_{nm} P_m(t') \tag{4.16}$$

where the rate constant is now approximated by

$$R_{nm} = \epsilon^2 \int_{-\infty}^{\infty} d\tau \, \exp[i\lambda(n - m)\tau] \langle Z_{nm}^*(\tau) Z_{nm}(0) \rangle \langle U_{mm}(\tau) \rangle$$

$$= \epsilon^2 f(n - m) \int_{-\infty}^{\infty} d\tau \, \exp[i\lambda(n - m)\tau] \, C(\tau) c(\tau) \tag{4.17}$$

where $c(\tau) = \langle U_{mm}(\tau) \rangle$. Note that this is in the same form as the perturbative expression for the rate constant (4.12), except that it involves a correlation function of both the $Z_{nm}$ and the $a_n$ variables. We do not claim that all of the steps in (4.16) can be strictly justified: our aim was to produce a simple model of the non-perturbative solution of (4.2) for further discussion. The long-time behaviour of (4.2) will be studied in detail in a subsequent paper.

## 5. Implications for the Schrödinger equation

We now transcribe the results of section 4 to the case of the adiabatic form of the Schrödinger equation (2.3). If the stochastic differential equation (4.2) is a good model for the Schrödinger equation, then the occupation probabilities are expected to obey the equation of motion (4.11), with rate constants obtained from (4.17):

$$R_{nm} = \dot{X}^2 \frac{\sigma^2(\Delta E)}{\Delta E^2} \int_{-\infty}^{\infty} d\tau \, \exp[i\Delta E\tau/\hbar] \, C(\tau) \, c(\tau) \tag{5.1}$$

where $\Delta E = E_n - E_m \approx (n-m)/\rho$. Approximating the summation in (4.15) by an integral, the diffusion constant is therefore

$$D = \tfrac{1}{2}\rho^3 \dot{X}^2 \int_{-\infty}^{\infty} d\Delta E \, \sigma^2(\Delta E) \int_{-\infty}^{\infty} d\tau \, \exp[i\Delta E\tau/\hbar] \, C(\tau) \, c(\tau)$$

$$= \tfrac{1}{2}\rho^3 \dot{X}^2 \int_{-\infty}^{\infty} d\Delta E \, \sigma^2(\Delta E) \, F(\Delta E) \tag{5.2}$$

where the second equality defines $F(\Delta E)$. The function $F(\Delta E)$ decays rapidly to zero when $\Delta E \gg \hbar/\tau_c$, where $\tau_c$ is the timescale for the decay of correlations of the matrix elements:

$$\tau_c \sim 1/\rho\sigma_0\dot{X} . \tag{5.3}$$

The total weight of the function $F(\Delta E)$ is

$$\int_{-\infty}^{\infty} d\Delta E \, F(\Delta E) = \int_{-\infty}^{\infty} d\tau \, C(\tau) \, c(\tau) \int_{-\infty}^{\infty} d\Delta E \, \exp[i\Delta E\tau/\hbar]$$

$$= 2\pi\hbar \int_{-\infty}^{\infty} d\tau \, \delta(\tau) \, C(\tau) \, c(\tau) = 2\pi\hbar \, C(0) \, c(0) = 2\pi\hbar \tag{5.4}$$

since, from (4.3) and (4.17), $C(0) = c(0) = 1$. If the support $\Delta E_0$ of $\sigma^2(\Delta E)$ is large compared to that of $F(\Delta E)$, then the diffusion constant can be approximated as follows:

$$D = \tfrac{1}{2}\rho^3 \dot{X}^2 \int_{-\infty}^{\infty} d\Delta E \, \sigma^2(\Delta E) \, F(\Delta E)$$

$$\sim \tfrac{1}{2}\rho^3 \dot{X}^2 \sigma_0^2 \int_{-\infty}^{\infty} d\Delta E \, F(\Delta E) = \pi\hbar\rho^3\sigma_0^2\dot{X}^2 . \tag{5.5}$$

Comparison with (1.3), (1.6) and (1.7) shows that this result gives a rate of dissipation which is, remarkably, exactly in agreement with the Kubo formula. The condition for this formula to hold is

$$\Delta E_0 \gg \hbar\rho\sigma_0\dot{X} \tag{5.6}$$

i.e. $\eta \ll 1$. In the opposite limit, when the scale size of the function $F(\Delta E)$ is large compared to that of $\sigma^2(\Delta E)$, a different prediction for the diffusion constant applies:

$$D \sim \rho^3\sigma_0^2\Delta E_0\hbar\dot{X}^2/\tau_c \sim \rho^2\sigma_0\Delta E_0\dot{X} . \tag{5.7}$$

The analogy between the stochastic differential equation (4.2) and the Schrödinger equation in the form (2.3) therefore suggests that there is a crossover between two regimes, characterized by the dimensionless parameter $\eta$. When $\eta \ll 1$, the Kubo formula is expected to apply, but when $\eta \gg 1$, the diffusion constant is predicted to be proportional to $\dot{X}$ instead of $\dot{X}^2$.

We now consider the extent to which these predictions are likely to be borne out in the usual Schrödinger equation. The approximations made in setting up the stochastic differential equations (4.2) as a model for the adiabatic Schrödinger equation (2.3) are all reasonable, but we must consider to what extent the diffusion of the adiabatic amplitudes $a_n(t)$ represents a real dynamical process, and to what extent it is reversible if the parameter $X(t)$ is returned to its original value. In section 2, it was noted that the equation of motion for a fixed state vector, (2.5), is similar to (2.3), differing only by a phase factor. Consider the change in the phase factors $\theta_n - \theta_m$ on the timescale $\tau_c$ over which the amplitudes $a_n(t)$ vary. If all of these phases are small for pairs of states close enough in energy that the matrix elements are significant, then the dynamics will be very close to that of a fixed state vector, (2.5). The condition for this is $\Delta E_0 \tau_c \ll \hbar$, and using the estimate for $\tau_c$ given by (5.3) this reduces to

$$\eta \gg 1. \tag{5.8}$$

When $\eta \gg 1$, we therefore expect that the diffusion constant predicted by (5.7) will overestimate the rate of dissipation.

We must also consider the extent to which the diffusion of occupation probabilities is reversible. We argued in section 2 that the diffusion is reversible if the matrix elements of the evolution operator are real, but that if the imaginary parts of the evolution operator are comparable to the real parts, the dynamics is irreversible. We will now present a heuristic argument for a criterion to determine in which limits the motion is reversible. We consider the situation in which the coordinate $X(t)$ is increased linearly from 0 at a rate $\dot{X}$ until it reaches $X_0$ at time $T$, and is then decreased linearly to return to 0 at $2T$. We also assume that the function $\sigma^2(\Delta E)$ is very small for energy differences larger than $\Delta E_0$. The phases $\theta_n - \theta_m$ appearing in (2.3) will therefore be small for all of the terms appearing in the sum with significant weight if the following condition is met:

$$\mu = \Delta E_0 T / \hbar \ll 1. \tag{5.9}$$

If equation (5.9) is satisfied, the imaginary parts of the elements of the evolution operator are small, and the motion is reversible. If $\Delta E_0 T / \hbar \gg 1$, there is no reason to assume that the imaginary parts of the matrix elements are small compared to the real parts, and we conclude that the motion is not reversible.

Our analysis of the stochastic differential equation model therefore leads to the following predictions about the dynamics when the perturbation strength is large, i.e. when $\chi \gg 1$. We predict that the Kubo formula estimate only applies if $\eta$ is small. If $\eta \gg 1$, the diffusion rate $D$ is reduced from the estimate $D_0$ obtained using the Kubo formula: our model predicts that $D/D_0 = O(1/\eta)$ when $\eta \gg 1$. The qualitative arguments above indicate that our model overestimates $D$ in this regime, and that if $\mu = \chi/\eta$ is small, the diffusion is reversible, whereas if $\mu \gg 1$ it is irreversible.

## 6. Numerical experiments on a time-dependent Hamiltonian

The discussion presented above is based on the assumption that the stochastic differential equation discussed in section 4 is a good model for the adiabatic Schrödinger equation.

Because this assumption is difficult to test analytically, we performed some numerical experiments on a 'real' time-dependent Schrödinger equation.

We considered a Hamiltonian of the form $\hat{H}(X) = \hat{H}_0 + \hat{V}(X)$, where the operators are represented by $N \times N$ matrices: $\hat{H}_0$ is a diagonal matrix with elements $H_{ij} = \alpha i \delta_{ij}$, and $\hat{V}(X)$ is a real symmetric band random matrix. The elements $V_{ij}$ of $\tilde{V}$ are (apart from the constraint $H_{ij} = H_{ji}$) independently Gaussian distributed, with mean and variance

$$\langle V_{ij} \rangle = 0 \qquad \langle V_{ij}^2 \rangle = \begin{cases} 1 + \delta_{ij} & |i - j| \leqslant b \\ 0 & |i - j| > b. \end{cases} \qquad (6.1)$$

The motivation for this choice of $\hat{H}$ is that these band random matrices have a structure similar to that of a perturbation of a typical complex quantum system [15].

Two different approaches were used to introduce a parameter dependence into the model. The first method was to simply combine two fixed realizations of the random matrix, $\hat{V}_1$ and $\hat{V}_2$, as follows:

$$\hat{H}(X) = \hat{H}_0 + \cos X \, \hat{V}_1 + \sin X \, \hat{V}_2. \qquad (6.2)$$

Note that the linear combination (6.2) has the same statistical properies for all values of $X$, and that the derivatives of the matrix elements are a band random matrix with the same statistical properties as $\hat{V}(X)$, i.e.

$$\left\langle \frac{dH_{ij}}{dX} \right\rangle = 0 \qquad \left\langle \left( \frac{dH_{ij}}{dX} \right)^2 \right\rangle = \begin{cases} 1 + \delta_{ij} & |i - j| \leqslant b \\ 0 & |i - j| > b. \end{cases} \qquad (6.3)$$

Also, note that the matrix $d\hat{H}/dX$ is statistically independent of $\hat{H}$.

The second method for introducing a parameter dependence was to obtain the matrix elements of $\hat{V}(X)$ by smoothing a white noise function:

$$V_{ij}(X) = \int_{-\infty}^{\infty} dX' \, W_{ij}(X') \, K(X - X'). \qquad (6.4)$$

Here the $W_{ij}(X)$ are uncorrelated white noise signals

$$\langle W_{ij}(X) W_{i'j'}(X') \rangle = \delta_{ii'} \, \delta_{jj'} \, \delta(X - X') \qquad (6.5)$$

and $K(x)$ is a smooth function (we used a Gaussian, with mean and variance chosen so that both (6.1) and (6.3) are satisfied). The integral in (6.4) was approximated by a summation over a set of uncorrelated random numbers representing the function $W_{ij}(X)$. The motivation for considering the more elaborate model (6.4) is that it allows us to study the effect of an arbitrarily large perturbation. In the version given by (6.2), the parameter dependence is periodic, so that the maximum excursion of $X(t)$ is effectively $\pi$.

An important property of this model, which we will refer to later, concerns the localization properties of the eigenfunctions. It is possible to argue persuasively that the localization length $L$ satisfies a scaling relationship of the form

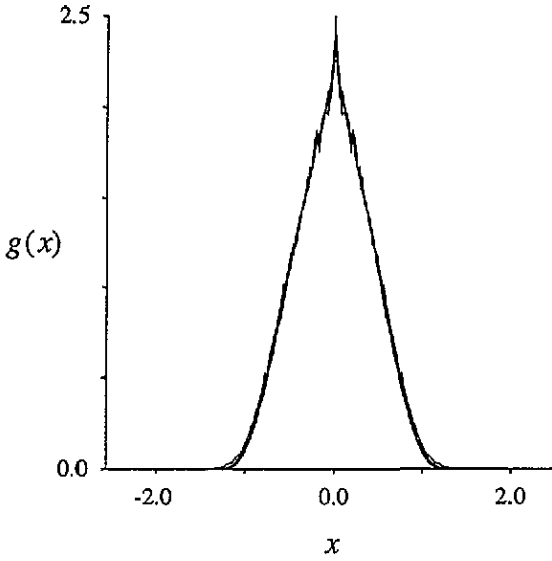$$L = b^2 \, f(\alpha b^{3/2}) \qquad (6.7)$$

**Figure 1.** Scaling function $g(x) = G(x, \gamma_0)$ characterizing the variance of the matrix elements for $\gamma_0 = 5$. Three curves are superposed, for data with $b = 7$, 10 and 15.

in the limit $N \rightarrow \infty$ [15]. In this limit, the density of states $\rho$ is

$$\rho = 1/\alpha \tag{6.8}$$

except close to the edge of the spectrum.

In order to use this model we require some information about the function $\sigma^2(\Delta E)$ which characterizes the matrix elements of $\partial \hat{H}/\partial X$ in the basis formed by the eigenfunctions of $\hat{H}(X)$. In the appendix we provide a heuristic argument indicating that this function satisfies the scaling relation

$$\sigma^2(\Delta E) = \frac{1}{b} G(\Delta E/\gamma b^{1/2}, \gamma) \qquad \gamma = \alpha b^{3/2} \tag{6.9}$$

where $G(x, y)$ is some unknown function. The form of (6.9) suggests that it is convenient to work at some fixed value of $\gamma$; we used $\gamma_0 = 5$ throughout. Figure 1 shows a plot of the function $\sigma^2(\Delta E)$ for various values of the bandwidth $b$, scaled in accordance with (6.9). These points lie close to the same curve $g(x) = G(x, \gamma_0)$ for all the values of $b$, confirming that the scaling relation (6.9) is a good approximation. We found that the results for different values of $b$ were however noticably different, and our results indicate that these differences are more probably due to a systematic finite size effect than to insufficient numerical averaging. We therefore took account of these differences when estimating the values of $\sigma_0$ and $\Delta E_0$. These quantities depend on the following two quantities which are obtained from the empirically determined function $g(x)$:

$$g_0 = g(0) \qquad I = \int_0^\infty dx \, g(x). \tag{6.10}$$

The values of $g_0$ and $I$ are given in table 1, for various values of $b$.

**Table 1.** Parameters used to calculate $\sigma_0$ and $\Delta E_0$ in the random matrix models, for various bandwidths $b$.

| $b$ | $g_0$ | $l$ |
|---|---|---|
| 5 | 2.66 | 1.397 |
| 7 | 2.15 | 1.093 |
| 8 | 2.41 | 1.106 |
| 10 | 2.27 | 1.098 |
| 12 | 2.47 | 1.097 |
| 15 | 2.39 | 1.056 |
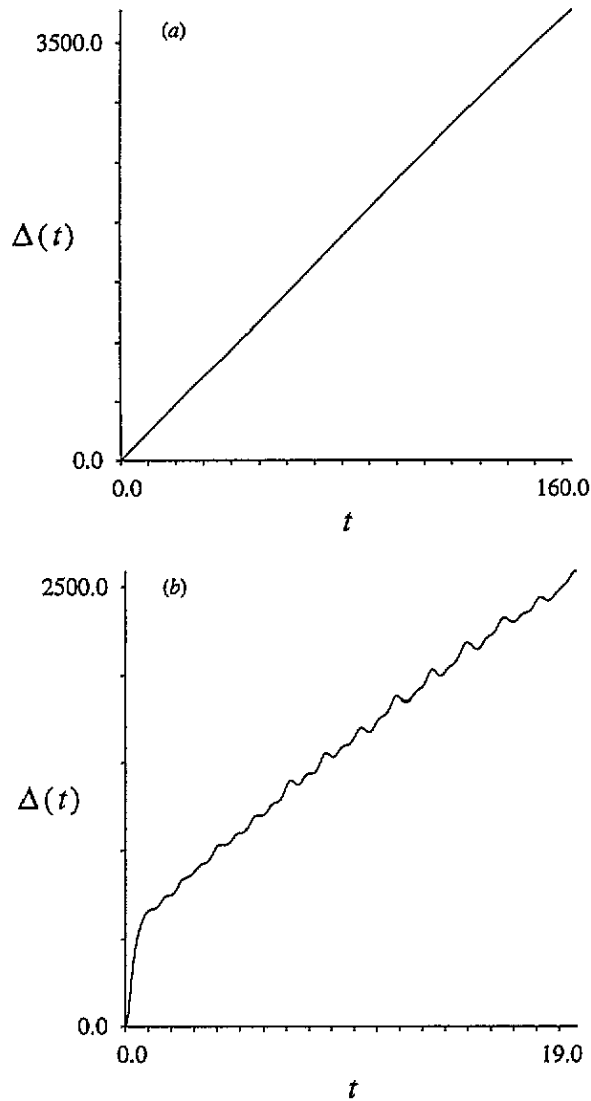


**Figure 2.** Second moment of energy distribution $\Delta(t)$ as a function of time. (*a*) corresponds to a small value of $\eta$, and (*b*) to a large value of $\eta$ where there is linear growth after an initial transient.

We investigated the dynamics by integrating the time-dependent Schrödinger equation using a fourth-order Runge–Kutta method. We transformed the wavefunction into the adiabatic basis at regular time intervals, and evaluated the mean value of the second moment (1.2). For all of our simulations we again set $\gamma = 5$. We chose the dimension $N$ such that $N \geqslant 4b^2$, and averaged over states in only the central third of the spectrum so as to avoid end effects, where (6.7)–(6.9) are not valid. When the scaling parameter $\eta$ is small, we find a linear growth of the second moment until this quantity starts to experience the constraints imposed by a finite-size matrix. When $\eta$ is large, the second moment initially grows rapidly (and apparently not linearly), and then continues growing linearly at a reduced rate. Figure 2 shows two typical examples, both for the model (6.2) with the parameter $X(t)$ inceasing linearly: (*a*) is for $b = 10$, $\dot{X} = 0.25$, corresponding to $\eta = 0.096$, and (*b*) is for $b = 8$, $\dot{X} = 4$, corresponding to $\eta = 1.53$.

The conclusions of section 5 suggest that the diffusion constant may satisfy a scaling relation of the form

$$D = D_0 \, f(\eta) \tag{6.11}$$

where $D_0$ is the diffusion constant predicted by (5.5), which gives results in agreement with the Kubo formula. We tested this hypothesis for the version of the model in which the matrix elements were obtained by smoothing a white noise signal, (6.4). The results are displayed in figure 3: they show a good fit to a scaling function $f(\eta)$ which approaches unity in the limit $\eta \to 0$. In the large $\eta$ regime, the function $f(\eta)$ decreases much faster than $1/\eta$; this is consistent with the arguments indicating that (5.7) is an upper bound.
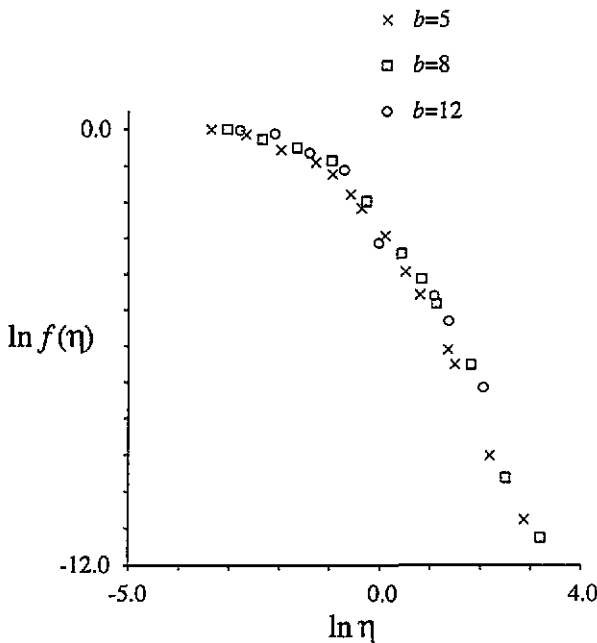


**Figure 3.** Logarithmic plot of the ratio $f$ of the actual diffusion constant $D$ to the Kubo formula prediction $D_0$, as a function of the scaling variable $\eta$. These data are from the model (6.4). The different types of point refer to different values of the bandwidth $b$.
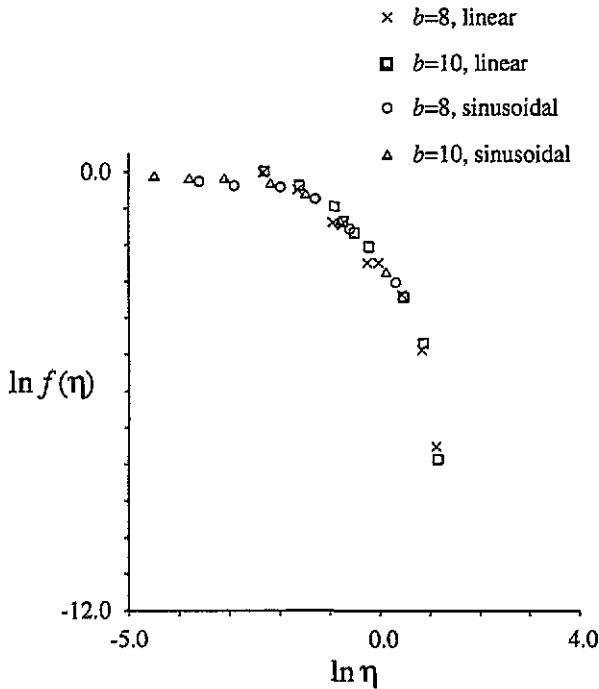
**Figure 4.** Same as for figure 3, showing data for model (6.2), for various values of $b$, and two different forms of the time dependence of the parameter $X(t)$.

We also investigated whether the scaling relationship holds for the model (6.2): the results are displayed in figure 4. Again there is a good fit to a scaling curve, and the function $f(\eta)$ is very close to that for (6.4) up to $\eta \approx 2$, but then falls away more rapidly. This plot shows data for both linear and sinusoidal $X(t)$; in the sinusoidal case we kept $X_0 b = $ constant $= 8$, in order to keep the dimensionless parameter $\chi$ constant. The fact that the scaling function decreases more rapidly as $\eta \to \infty$ is consistent with the discussion at the end of section 5, which indicates that the effects of the perturbation are reversible if $\mu = \chi/\eta$ is small: recall that $\chi$ is finite for (6.2) but it has unbounded growth for (6.4).

## 7. Estimates of dimensionless parameters

It is important to understand how the dimensionless parameters which characterize the dynamics scale as a function of the physical parameters of the system. It will be shown that $\eta$ can be very large in situations of physical interest. Two examples will be considered.

### 7.1. The semiclassical limit

Here we consider the limit $\hbar \to 0$, with all classical quantities held fixed. For definiteness, we assume that the system is subjected to a periodic perturbation of frequency $\omega$, and amplitude $X_0$, and that the scale size of the effect of the perturbation on a typical trajectory is characterized by an energy $\delta E$. The variance of the matrix elements is related to the classical correlation function of the perturbation as follows [13]:

$$\sigma^2(\Delta E) = \frac{1}{2\pi\rho\hbar} \int_{-\infty}^{\infty} \mathrm{d}t \, \exp[\mathrm{i}\Delta E t/\hbar] \left\langle \frac{\partial H}{\partial X}(t) \frac{\partial H}{\partial X}(0) \right\rangle_{\mathrm{cl}}. \tag{7.1}$$

This leads to the estimates

$$\sigma_0 X_0 \sim \delta E \sqrt{\frac{\tau_{\text{cl}}}{\rho \hbar}} \qquad \Delta E_0 \sim \hbar/\tau_{\text{cl}} \tag{7.2}$$

where $\delta E$ is the typical magnitude of the perturbation of the classical Hamiltonian, and $\tau_{\text{cl}}$ is the timescale for the decay of classical correlations. From these results, the parameter $\eta$ can be estimated as follows:

$$\eta \sim \tau_{\text{cl}} \, \omega \, \rho \, \delta E \sqrt{\frac{\tau_{\text{cl}}}{\rho \hbar}} \, . \tag{7.3}$$

It is useful to write this in terms of the quantum number (the number $\mathcal{N}(E)$ of states below the energy $E$): clearly $\mathcal{N} \sim \rho E$, and from the Weyl rule [2] $\mathcal{N} \sim (E\tau_{\text{cl}}/\hbar)^d$, where $d$ is the number of degrees of freedom. This gives

$$\eta \sim \omega \, \tau_{\text{cl}} \frac{\delta E}{E} \mathcal{N}^{(d+1)/2d} \, . \tag{7.4}$$

From equations (7.3) or (7.4) it is clear that $\eta \to \infty$ in the semiclassical limit ($\hbar \to 0$ or $\mathcal{N} \to \infty$). A similar argument [3, appendix B] shows that $\chi \to \infty$ in the semiclassical limit. These results imply that the parameter regime corresponding to the semiclassical limit corresponds to the regime in which our model shows behaviour at variance with the Kubo formula.

### 7.2. Electrical conductance of a loop

We now show that $\eta$ can be large in the thermodynamic limit, taking electrical conduction as a specific example. In the case of a loop of material threaded by a magnetic flux, the DC conductance at zero temperature is obtained by setting $\omega = 0$ in (1.6):

$$\Sigma(0) = \pi \hbar \rho^2 \sigma^2(E_{\text{F}}, 0) \, . \tag{7.5}$$

Using the generalized Landauer formula [16], the DC conductance can also be written in the form

$$\Sigma(0) = \frac{e^2}{h} \, \text{tr}(\hat{t}^+ \hat{t}) \equiv \frac{e^2}{h} N_{\text{ch}} \tag{7.6}$$

where $\hat{t}$ is the transmission matrix for propagation around the loop at the Fermi energy, and the second equality defines the effective number of channels, $N_{\text{ch}}$.

Combining these results, and using the estimate $\Delta E_0 \sim \hbar \tau_{\text{r}}$, where $\tau_{\text{r}}$ is the relaxation time for scattering, our estimate for the parameter $\eta$ is

$$\eta \sim \frac{e \tau_{\text{r}}}{h} \dot{\Phi} \sqrt{N_{\text{ch}}} \, . \tag{7.7}$$

If the relaxation time is $\tau_{\text{r}} \sim 10^{-13}$ s, and the EMF is $\dot{\Phi} \sim 1$ V, the parameter $\eta$ is approximately 40 when $N_{\text{ch}} = 1$, and it is very large in a good conductor, for which $N_{\text{ch}} \gg 1$.

Because the energy levels are periodic in the flux $\Phi$, with period one flux quantum ($h/e$), the effective amplitude of the perturbation is $\Phi_0 \sim h/e$. Comparison with (7.5) and (7.6) shows that the dimensionless perturbation strength is

$$\chi = \rho \sigma_0 \Phi_0 \sim \sqrt{N_{\text{ch}}} \tag{7.8}$$

which is large for a good conductor. Once again, a situation of physical interest corresponds to a large value of both the parameters $\eta$ and $\chi$.

## 8. Discussion

We have considered the response of a complex quantum system, modelled by a random matrix, to a perturbation satifying $\chi \gg 1$: such a perturbation is large enough to cause mixing of energy levels, but could be very small on a classical scale. The response was characterized by examining the second moment of the energy distribution, which has a linear growth, proportional to the dissipation of energy in a system of independent fermions. We found that the dynamics of the system can be characterized by a dimensionless parameter $\eta$, and that if $\eta \gg 1$, the diffusion constant is less than that required to give a rate of dissipation consistent with the Kubo formula. These results were predicted using a stochastic differential equation which was devized to simulate the adiabatic form of the Schrödinger equation, and subsequently verified by simulations using the time-dependent Schrödinger equation of a random matrix model.

Estimates of the value of the parameter $\eta$ indicate that it is typically large in situations where the spacing between energy levels is extremely small. Two cases were considered: the semiclassical limit, and electrical conduction in a metallic ring. We have therefore shown that, in the case of our random matrix model, the Kubo formula fails in a parameter regime which corresponds to typical physical applications.

There are strong arguments which indicate that the predictions of our model for the large $\eta$ limit are not universally applicable. In the case of the semiclassical limit, the diffusion constant can be calculated from classical dynamics, and it gives a rate of dissipation which agrees precisely with Kubo formula [3]. In the example of conduction in a ring, our results would indicate a breakdown of Ohm's law at a critical voltage $\dot{\Phi}$ where $\eta \sim 1$, and the results of section 7.2 indicate that this critical voltage is extremely small for a good conductor. This is, of course, at variance with what is observed experimentally.

Two significant conclusions can be drawn from our results, one concerning the Kubo–Greenwood formula, the other concerning the use of random matrix models. Our first conclusion is that, in a non-perturbative regime, the Kubo–Greenwood formula is not universally applicable, because it fails for our random matrix model. The conditions for the validity of this formula in the physically relevant non-perturbative regime therefore need to be carefully examined.

The second conclusion is that our random matrix model gives unphysical results when applied to the dynamics of some complex systems; we have discussed electrical conduction in a loop and semiclassical systems as two examples. Random matrix models have been very successful in describing the spectra of complex systems; it is natural to extend them to dynamical properties, by hypothesizing that the dynamics resemble those of random matrix models after scaling the parameters appropriately. The results of this paper indicate that, if there are 'universal' models for the dynamics of complex systems based on random matrices, they must represent additional properties of the Hamiltonian which are not included in our model. We can suggest what some of these additional properties might be: in semiclassical systems, matrix elements satisfy sum rules which imply that they are correlated [17]; in models for electrical conduction, such as the Anderson model, the Hamiltonian acts 'locally' in space. It is probable that these features can explain the discrepancy between the dynamics of real systems and our random matrices. The nature and extent of this discrepancy is a problem for further research.

### Acknowledgments

carried out, and the Institute for Scientific Interchange in Turin, where this paper was completed.

## Appendix

Here we produce a heuristic argument to justify the scaling relation (6.9) for the variance $\sigma^2(\Delta E)$ of the matrix elements $\langle \phi_n | \partial \hat{H} / \partial X | \phi_m \rangle$ of the models discussed in section 6.

For both versions of our random matrix model the matrix $d\hat{H}/dX$ is a banded random matrix, statistically independent of $\hat{H}(X)$. The matrix elements of $d\hat{H}/dX$ have the same variance (given by (6.3)) as those of $\hat{H}(X)$, but with the mean value of all the matrix elements equal to zero. In order to characterize the required matrix elements, we need some information about the eigenstates. If $b \gg 1$, and $N \gg b^2$, we can reasonably model the $j$th component of the $i$th eigenvector as a Gaussian distributed random number $v_j^i$ with statistical properties defined by

$$\langle v_j^i \rangle = 0 \tag{A.1}$$

$$\langle v_j^i v_{j'}^{i'} \rangle = \delta_{ii'} \, \delta_{jj'} \, h(i - j). \tag{A.2}$$

The function $h(i - j)$ is assumed to decay to zero rapidly as $|i - j| \to \infty$, reflecting the fact that the eigenstates are localized. The second moment of the function $h(n)$ can be indentified with the square of the localization length, $L$, which is given by (6.7). Normalization of the eigenvectors implies that

$$\sum_{n=-\infty}^{\infty} h(n) = 1. \tag{A.3}$$

We now estimate $\sigma^2$ in terms of this model: the matrix elements we require are

$$\langle \phi_n | \partial \hat{H} / \partial X | \phi_m \rangle = \sum_i \sum_j v_i^n \left( \frac{dH}{dX} \right)_{ij} v_j^m \tag{A.4}$$

and their variance is

$$\left\langle \left| \langle \phi_n | \frac{\partial \hat{H}}{\partial X} | \phi_m \rangle \right|^2 \right\rangle = \sum_i \sum_j \sum_k \sum_l \left\langle \left( \frac{dH}{dX} \right)_{ij} \left( \frac{dH}{dX} \right)_{kl} \right\rangle \langle v_i^n v_j^m v_k^n v_l^m \rangle$$

$$= \sum_i \sum_{j=i-b}^{i+b} \langle (v_i^n)^2 \rangle \langle (v_j^m)^2 \rangle = \sum_i \sum_{j=i-b}^{i+b} h(n - i) \, h(m - j)$$

$$= \sum_i h(i) \sum_{j=m-n+b+i}^{m-n-b+i} h(j) = \sigma^2(n - m) \tag{A.5}$$

where the last equality defines the function $\sigma^2(n)$.

First we make a crude estimate of $\sigma^2(0)$, which gives the variance of matrix elememts at or close to the diagonal. Because the localization length (which is $O(b^2)$) is large compared to $b$, we can approximate $\sigma^2(0)$ as follows:

$$\sigma^2(0) = \sum_i \sum_{j=i-b}^{i-b} h(i) \, h(j) \sim (2b + 1) \sum_n [h(n)]^2. \tag{A.6}$$

The normalization property (A.3) implies that there are $\sim L$ of the $h(n)$ which are significantly different from zero, and that these elements have typical size $\sim 1/L$. Hence (A.6) and (6.7) imply that

$$\sigma^2(0) \sim \frac{b}{L} \sim \frac{1}{bf(\gamma)} . \tag{A.7}$$

It is clear from (A.5) that the matrix elements are small if $|n - m| \gg L$, because both of the $h(n)$ terms will be small. This implies that the matrix elements will be small if $\Delta E \gg L/\rho = \alpha L$. These considerations therefore suggest the following scaling relation for the function $\sigma^2(\Delta E)$:

$$\sigma^2(\Delta E) = \frac{1}{bf(\gamma)} \Gamma\left(\Delta E/\alpha b^2 f(\gamma)\right) \tag{A.8}$$

for some unknown scaling function $\Gamma(x)$. This can also be expressed in the form

$$\sigma^2(\Delta E) = \frac{1}{b} G\left(\Delta E/\alpha b^2, \gamma\right) \tag{A.9}$$

where $G(x, \gamma)$ is a function which is a symmetric function of $x$ which is expected to have a value of order unity at $x = 0$, and to decay rapidly for values of $x$ large compared to unity.

## References

[1]   Porter C E (ed) 1965 *Statistical Theories of Spectra: Fluctuations* (New York: Academic)
[2]   Gutzwiller M C 1990 *Chaos in Classical and Quantum Mechanics* (New York: Springer)
[3]   Wilkinson M and Austin E J 1992 *Phys. Rev.* A 46 64–74
[4]   Wilkinson M 1990 *Phys. Rev.* A 41 4645–52
[5]   Chirikov B, Shepelyansky D L and Izraelev F 1981 *Sov. Sci. Rev.* C 2 209
[6]   Wilkinson M 1988 *J. Phys. A: Math. Gen.* 21 4021–37
[7]   Kubo R 1956 *Canadian J. Phys.* 34 1274–7
[8]   Greenwood D A 1958 *Proc. Phys. Soc.* A 68 585–96
[9]   van Kampen N G 1971 *Acta Phys. Norvegica* 5 279–84
[10]  Shapere A and Wilczek F (eds) 1989 *Geometric Phases in Physics* (Singapore: World Scientific)
[11]  Pechukas P 1983 *Phys. Rev. Lett.* 51 943–6
[12]  Austin E J and Wilkinson M 1992 *Nonlinearity* 5 1137–50
[13]  Wilkinson M 1987 *J. Phys. A: Math. Gen.* 20 2415–23
[14]  Yukawa T 1985 *Phys. Rev. Lett.* 54 1883
[15]  Wilkinson M, Feingold M and Leitner D M 1991 *J. Phys. A: Math. Gen.* 24 175–82
[16]  Fisher D S and Lee P A 1981 *Phys. Rev.* B 23 6851–4
[17]  Wilkinson M 1988 *J. Phys. A: Math. Gen.* 21 1173–90