Diffusion and dissipation in complex quantum systems

Michael Wilkinson
Department of Physics and Applied Physics, John Anderson Building, Strathclyde University, Glasgow G4 ONG, Scotland, United Kingdom
(Received 10 October 1989)

The Hamiltonian of a quantum-mechanical system contains a time-dependent parameter X. The system is prepared in a highly excited eigenstate of the instantaneous Hamiltonian at $t=0$, and we compute the amplitudes $\langle n(t)|\psi(t)\rangle$ to be in the eigenstates $|n\rangle$ of the instantaneous Hamiltonian $\hat{H}(X(t))$ at later times. It is found that for generic systems, with no symmetries yielding additional quantum numbers, the occupation probability spreads diffusively away from the initial state. This diffusion is an irreversible process, and can be related to a model for dissipation. The diffusion constant D is investigated numerically in a random matrix model as a function of $\dot{X}$, the rate of change of the parameter. Good agreement with theoretical predictions is found in two limiting regimes. When $\dot{X}$ is large, D is proportional to $\dot{X}^2$, corresponding to the Ohmic dissipation predicted by the Kubo formula. When $\dot{X}$ is small, Landau-Zener transitions are the mechanism for diffusion, and D is proportional to $\dot{X}^{3/2}$.

I. INTRODUCTION

A quantum-mechanical system has a Hamiltonian $\hat{H}(X)$ depending on a parameter X. The parameter X is time dependent, and varies at a rate $\dot{X}$. Initially, the state $|\psi\rangle$ is a highly excited eigenstate of the instantaneous Hamiltonian at $t=0$, i.e.,

$$|\psi(0)\rangle=|n(0)\rangle\ , \tag{1.1}$$

where

$$\hat{H}(X(t))|n(t)\rangle=E_n(X(t))|n(t)\rangle\ . \tag{1.2}$$

We consider the evolution of the state $|\psi(t)\rangle$, expressed in a basis of the eigenstates of the instantaneous Hamiltonian

$$|\psi(t)\rangle=\sum_m a_m(t)|m(t)\rangle\ . \tag{1.3}$$

The motivation for this choice of basis is that if the state evolves adiabatically, then the $|a_m(t)|$ do not change.

In a broad class of systems (which will be discussed later), the occupation probability spreads diffusively: if we characterize the time evolution by the second moment of the probability distribution

$$\Delta_n(t)=\sum_m |a_m(t)|^2(m-n)^2\ , \tag{1.4}$$

it is found that $\Delta_n(t)$, averaged over many states, exhibits a diffusive growth, i.e.,

$$\langle\Delta(t)\rangle=2Rt\ . \tag{1.5}$$

This paper will describe the results of numerical experiments where this diffusive behavior is observed, and where the dependence of the diffusion constant R on $\dot{X}$ is investigated.

A consequence of this diffusive behavior is that the coarse-grained occupation probability satisfies a diffusion equation. This quantity, denoted by $f(E)$, can be defined as follows:

$$f(E)=\frac{1}{\rho(E)}\sum_n |\langle\psi|n\rangle|^2\,\delta_\varepsilon(E-E_n)\ , \tag{1.6}$$

where $\delta_\varepsilon(x)$ is a distribution function centered on $x=0$, with a width ε which is large compared to the typical separation of energy levels, but small compared to other energy scales characterizing the system, and $\rho(E)$ is the smoothed density of states

$$\rho(E)=\sum_n \delta_\varepsilon(E-E_n)\ . \tag{1.7}$$

The probability density $f(E)$ satisfies a diffusion equation of the form

$$\frac{\partial(\rho f)}{\partial t}+\dot{X}\frac{\partial}{\partial E}\left[\frac{dE}{dX}\rho f\right]=\frac{\partial}{\partial E}\left[D\rho\frac{\partial f}{\partial E}\right]\ . \tag{1.8}$$

The drift term proportional to $\dot{X}$ on the left-hand side of (1.8) takes account of the variation of $f(E,t)$ due to the change in the energy levels with the parameter X. In this expression dE/dX is the local average rate of variation of an energy level with respect to X, which could be defined by analogy with (1.6):

$$\frac{dE}{dX}=\sum_n \frac{dE_n}{dX}\delta_\varepsilon(E-E_n)\ . \tag{1.9}$$

This diffusion equation is consistent with (1.5) if the diffusion constants D and R are related by

$$D=R/\rho^2\ . \tag{1.10}$$

The diffusive spread of occupation probability is an irreversible process: we do not recover the original state $|\psi(0)\rangle$ by reversing the sign of $\dot{X}$ and returning to the original Hamiltonian. The diffusion of occupation probability is of physical interest because it is closely related to

a model for the microscopic mechanism of dissipation, another irreversible process, which will be discussed in Sec. II.

Theoretical predictions[1] of the size of the diffusion constant and its dependence on $\dot{X}$ are described in Sec. III. Much of this theory uses random matrix models for the statistical properties of the spectrum of the system. The use of these models is described in a reprint volume edited by Porter,[2] and is justified for most complex quantum systems which do not have extra constants of motion leading to additional quantum numbers.[3] The numerical work in this paper models systems which have time reversal invariance, for which the appropriate random matrix model is the Gaussian orthogonal ensemble (GOE). If there are constants of motion in addition to the energy, the predictions based on random matrix theory do not apply, and the occupation probability may not spread diffusively.

The numerical experiments were carried out using a parameter-dependent version of the GOE random matrix model. These numerical experiments are described in Sec. IV, and the results are found to be in good agreement with the theoretical predictions.

Even if the system is one for which random matrix theory gives a good description of the spectrum and the matrix elements, there may be other factors which limit the applicability of the results. Section V gives a further discussion of the types of system for which diffusion of the occupation probability will occur.

II. MODEL FOR DISSIPATION

The microscopic mechanism for dissipation is the transfer of energy from an observed degree of freedom to a large number of microscopic degrees of freedom. Often, it is assumed that the microscopic degrees of freedom can be modeled by a bath of harmonic oscillators, with a continuous spectrum of frequencies.[4] In this paper we consider a different situation: the oscillators are identical to each other, but they have complex dynamics, so that their quantum-mechanical dynamics can be described by random matrix theory and exhibits the diffusive behavior described in the Introduction. The parameter X which appears in the Hamiltonian is the observed degree of freedom, which couples to the oscillators independently. Usually, the microscopic oscillators would be a gas of weakly interacting fermions confined by a potential well, which can be deformed by varying the parameter X.

An example of a physical problem for which this would be a suitable model is the absorption of low-frequency electromagnetic radiation by small conducting particles. If the particles are irregularly shaped, the spectrum of the electrons (treated as a system of independent quasiparticles) is described by random matrix theory, and the electric field of the radiation plays the role of the time-dependent classical parameter X.

We characterize the dissipative process by calculating the irreversible component of the rate of change of the energy of the bath of oscillators as we vary the parameter X: by conservation of energy this is the rate at which the energy of the observed degree of freedom is dissipated. Typically, the observed degree of freedom experiences a dissipative force which is proportional to its velocity: this is often called viscous or Ohmic damping. In this case the power dissipated is proportional to the square of the velocity

$$\frac{dE}{dt}=\mu(X)\dot{X}^2 . \tag{2.1}$$

It will be shown that this form arises naturally for systems which show the diffusive behavior described above.

Our aim is therefore to calculate the rate of change of the energy of the system of oscillators. The expectation value of the energy of the system is initially

$$E_T=\sum_n |\langle\psi(0)|n\rangle|^2 E_n=\int_{-\infty}^{\infty} dE\, f(E,t)\rho(E)E . \tag{2.2}$$

When the system is perturbed by varying X, both the occupation probability $f(E,t)$ and the energy levels change. The time derivative of the expectation value of the energy is therefore [substituting (1.8) into (2.2) and integrating by parts]

$$\frac{dE_T}{dt}=\dot{X}\int_{-\infty}^{\infty} dE\,\rho f\frac{dE}{dX}+\int_{-\infty}^{\infty} dE\,\rho D\frac{\partial f}{\partial E} . \tag{2.3}$$

The first term on the right-hand side is proportional to $\dot{X}$, and represents a reversible change in the energy of the system. The second term represents the irreversible dissipation of energy. If the occupation probability f decreases very rapidly at the Fermi energy, (2.3) simplifies to

$$\frac{dE_T}{dt}=\dot{X}\int_{-\infty}^{E_F} dE\,\rho\frac{dE}{dX}+\rho_F D_F , \tag{2.4}$$

where $\rho_F=\rho(E_F)$, etc. From this result we see that the rate of dissipation is equal to the diffusion constant multiplied by the density of states, where both quantities are evaluated at the Fermi energy.

The mechanism of dissipation is therefore the diffusion of particles with energies at or just below the Fermi energy into states with energies above the Fermi energy. It might be thought that the Pauli principle would inhibit this diffusion, resulting in a reduced rate of dissipation. It is simple to show that this is not the case: see Appendix A for a discussion of this point.

III. THEORETICAL PREDICTIONS

The theoretical predictions for the diffusion constant depend on some properties of the matrix elements of the force operator $\partial\hat{H}/\partial X$ in a basis of eigenstates $|n\rangle,|m\rangle,\ldots$ of the Hamiltonian $\hat{H}$. If $\hat{H}$ has no symmetries or conserved quantities, these matrix elements are quasirandom, and we can discuss their statistical properties in terms of local averages within the matrix; for instance, the second moment of the off-diagonal matrix elements can be defined as

$$\sigma^2(E,\Delta E)=\left\langle \left| \left[\frac{\partial H}{\partial X}\right]_{nm}\right|^2\right\rangle_{\substack{E_n-E_m\simeq\Delta E \\ \frac{1}{2}(E_n+E_m)\simeq E}}$$

$$=\sum_{n,m}\left| \left[\frac{\partial H}{\partial X}\right]_{nm}\right|^2 \delta_\varepsilon(E-\tfrac{1}{2}(E_n+E_m))$$

$$\times\delta_\varepsilon(\Delta E-(E_n-E_m))\ , \tag{3.1}$$

where $\delta_\varepsilon(x)$ is a distribution function of width ε, which is large compared to the mean level spacing but small compared to the other energy scales of the system. In Appendix B it is shown that the matrix elements are locally independently Gaussian distributed, the mean value of the off-diagonal matrix elements is zero, and their variance σ^2 is a smooth function of E and ΔE. The diagonal matrix elements need not have a mean value of zero. Their variance is related to the variance of the nearby off-diagonal matrix elements $\sigma^2(E,0)$:

$$\left\langle \left| \left[\frac{\partial H}{\partial X}\right]_{nn}-\left\langle\left[\frac{\partial H}{\partial X}\right]_{nn}\right\rangle\right|^2\right\rangle_{E_n\simeq E}$$

$$=\beta\left\langle \left| \left[\frac{\partial H}{\partial X}\right]_{nm}\right|^2\right\rangle_{\substack{E_n\simeq E \\ E_m\simeq E}}$$

$$=\beta\sigma^2(E,0)\ , \tag{3.2}$$

where $\beta=2$ if the transformation which diagonalizes $\hat{H}$ is orthogonal (GOE case), and $\beta=1$ if it is unitary [Gaussian unitary ensemble (GUE) case]. The only statistic which plays a direct role in the theory for the diffusion constant $D(E)$ is $\sigma(E,0)$, (i.e., the variance of the near-to-diagonal matrix elements) which will be abbreviated to σ.

The diffusion constant is predicted to be a universal function of $\rho,\sigma,\hbar,\dot{X}$ for systems within a given universality class of the spectral statistics (Gaussian orthogonal, unitary, or symplectic ensembles)

$$D=\frac{1}{\rho^3\hbar}f_\beta(\rho^2\sigma\hbar\dot{X})=\frac{1}{\rho^3\hbar}f_\beta(\kappa)\ , \tag{3.3}$$

where f_β is a universal function depending only on the class of spectral statistics, labeled by the constant β appearing in (3.2). The dimensionless parameter $\kappa=\rho^2\sigma\hbar\dot{X}$ is a measure of the degree of adiabaticity (slowness) of the variation in the Hamiltonian. The asympotic form of the function $f_\beta(\kappa)$ can be calculated in both the limits of small and large κ, and these cases will be discussed separately.

When κ is small, the adiabatic theorem[5] is applicable, and the occupation probabilities remain constant except at values of X where two eigenvalues become very nearly degenerate, when occupation probability can be transferred by a Landau-Zener transition.[6] The points at which energy levels become very nearly degenerate (i.e., approach a separation ΔE which is much less than the mean level spacing $1/\rho$) are called avoided crossings, and they have the geometry of a hyperbolic section,[3] as illustrated in Fig. 1. Each avoided crossing is characterized by an energy gap ΔE and the difference A between the asymptotic slopes of the curves $E_n(X)$. If the wave function is initially in the nth level, the probability of making a nonadiabatic transition to the $(n+1)$th level is[6]

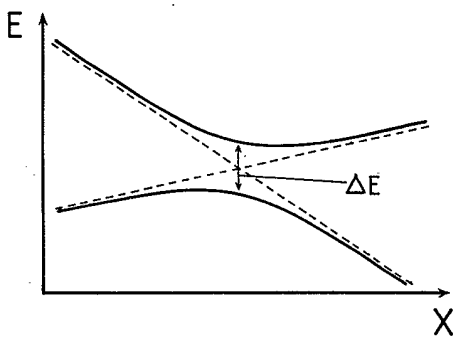

FIG. 1. For some values of X, pairs of energy levels become very nearly degenerate; these events are called avoided crossings. At these avoided crossings the adiabatic theorem breaks down, enabling diffusion of the probability density. The avoided crossing is characterized by the gap size ΔE and the difference A between the asymptotic slopes of the curves (dotted lines).

$$P_t=\exp(-\Delta E^2/\pi A\hbar\dot{X})\ . \tag{3.4}$$

If the occupation probabilities for the two states are initially P_n and P_{n+1}, then after the avoided crossing[1]

$$P_n'=P_n(1-P_t)+P_{n+1}P_t$$

$$+2[P_nP_{n+1}P_t(1-P_t)]^{1/2}\sin(\phi)\ , \tag{3.5}$$

and similarly for P_{n+1}', where ϕ is a phase which cannot be deduced from the parameters of the avoided crossings alone. The rate of diffusion of the occupation probability can be calculated analytically in the limit $\kappa\ll1$, by averaging (3.4) over the distribution of ΔE and A, assuming that ϕ is a random variable, so that the quantum interference term in (3.5) can be ignored. This has been done for the GOE and GUE cases; the results are[1]

$$f_2(\kappa)=2^{-5/4}\pi\Gamma(\tfrac{3}{4})\kappa^{3/2},\quad \text{GOE} \tag{3.6}$$

and

$$f_1(\kappa)=\pi\kappa^2,\quad \text{GUE}\ . \tag{3.7}$$

Because the transfer of occupation probability occurs in steps where there is a near degeneracy of eigenvalues, these results are only meaningful if many Landau-Zener transitions contribute to the diffusion, so that we may take a statistical average. The condition for this to be valid is that the predicted spread of the occupation probability is large compared to the mean separation of energy levels. The different power laws characterizing the κ dependence in (3.6) and (3.7) are a reflection of the fact that the GUE has stronger level repulsion than the GOE, so that there are fewer near degeneracies between energy

levels. The power law is related to the behavior of the level spacing distribution[2] $P(S)$ for small S: If $P(S) \propto S^{\nu}$ for small S, then $f(\kappa) \propto \kappa^{(\nu+2)/2}$ for small κ.[1] The GOE, GUE, and Gaussian symplectic ensemble (GSE) all have this property, with $\nu=1$, 2, and 4, respectively.

When $\kappa \gg 1$, the adiabatic theorem is not applicable, and Landau-Zener transitions are no longer the mechanism of diffusion. Instead, transitions are not restricted to nearest-neighboring states and may occur between pairs of states which differ in energy by $\Delta E < \rho\sigma\hbar\dot{X}$. The time scale for these transitions is $\tau \simeq \rho\hbar$, so that the diffusion constant is $D \simeq \Delta E^2/\tau$, i.e., $D \propto \kappa^2/\rho^3\hbar$. The multiplying constant can be deduced by comparison[1] with the rate of dissipation calculated using the Kubo-Greenwood formula,[7,8] which is derived assuming that the adiabaticity parameter $\kappa \gg 1$. The result is

$$f(\kappa)=\pi\kappa^2 , \tag{3.8}$$

independent of the universality class of the spectral statistics. The fact that the multiplying constant is the same in (3.7) and (3.8) appears to be a coincidence.

IV. NUMERICAL EXPERIMENTS

The theoretical predictions about the diffusion constant for time-reversal invariant systems were tested against numerical experiments on a random matrix model. The random matrix ensemble appropriate for describing the spectral statistics of these systems is the Gaussian orthogonal ensemble described by Porter.[2] Without loss of generality, we can define the GOE as follows: the matrix elements H_{ij} of a symmetric matrix of dimension N are independent Gaussian random variables with mean zero and variance

$$\mathrm{var}(H_{ij})=1+\delta_{ij} . \tag{4.1}$$

The density of states in this model is given by Wigner's semicircle law[2] in the limit of large N,

$$\rho(E)=\frac{\sqrt{N}}{\pi}(1-E^2/4N)^{1/2} . \tag{4.2}$$

A parameter dependence must be built into the model; this can be achieved by obtaining the matrix elements by smoothing a white-noise functions W_{ij} with an appropriate function f,

$$H_{ij}(X)=\int_{-\infty}^{\infty} dX' f(X-X')W_{ij}(X') , \tag{4.3}$$

so that the matrix elements are a smoothly varying function of X. The white-noise function has unit intensity and no correlations,

$$\langle W_{ij}(X)W_{i'j'}(X')\rangle=\delta_{ii'}\delta_{jj'}\delta(X-X')(1+\delta_{ij}) . \tag{4.4}$$

The matrix elements were obtained by a simple numerical integration of (4.3), in which the white-noise function W was simulated by an array of uncorrelated random numbers. The function $f(X)$ was chosen to be causal (zero for $X<0$) to facilitate this. The function chosen was

$$f(X)=\begin{cases} aX^2e^{-bX}, & X\geq 0 \\ 0, & X\leq 0 \end{cases} \tag{4.5}$$

which has one continuous derivative, and gives the matrix elements a continuous first derivative. The matrix $\partial H_{ij}/\partial X$ is also a representative of a Gaussian orthogonal ensemble. The following choice of the constants a and b in (4.5) makes the variance of the off-diagonal matrix elements of $\hat{H}$ and $\partial\hat{H}/\partial X$ equal to unity:

$$a=2\times 3^{3/4}, \quad b=\sqrt{3} . \tag{4.6}$$

It follows from the defining properties of the Gaussian orthogonal ensembles[2] that the matrix elements of $\partial\hat{H}/\partial X$ in the basis formed by the eigenvectors of $\hat{H}$ are also representative of a GOE with the same variance. The parameter σ is therefore equal to unity for this model.

Numerical experiments of the type described in the Introduction were performed using this model. The Schrödinger equation was integrated using a fourth-order Runge-Kutta method, and the coefficients a_m were found by projecting the wave function at regular time intervals onto eigenvectors of the instantaneous Hamiltonian, obtained by a standard diagonalization package. The spread of the wave function was characterized by evaluating the second moment of the occupation probability, (1.4). Especially in the limit of small adiabaticity parameter κ, the results had to be quite heavily averaged to show the diffusive behavior clearly; they were averaged over different realizations of the random matrix Hamiltonian and over different choices of the initial state $|\psi(0)\rangle=|n(0)\rangle$. The initial eigenstate was always chosen to be near the center of the spectrum, and the simulation was stopped before the wave function had spread into the tails of the spectrum, so that the density of states could be assumed to be a constant, equal to its value at $E=0$ [i.e., $\rho=\sqrt{N}/\pi$, cf. Eq. (4.2)]. For the model described above, we have $\hbar=\sigma=1$, so that Eqs. (1.10) and (3.3) become

$$\kappa=\frac{N\dot{X}}{\pi^2}, \quad R=\rho^2 D=\frac{\pi}{\sqrt{N}}f_2(\kappa) . \tag{4.7}$$

The diffusion constants R were estimated for two sizes of random matrices ($N=21$ and 45) for a range of values of $\dot{X}$. For the $N=21$ system, the evolutions of all initial states between $n=8$ and 12 were followed, and the values of $\Delta_n(t)$ averaged over these initial states and over ten different realizations of the random matrix. For the $N=45$ system the results were averaged over initial states from $n=15$ to 30, and over five realizations of the random matrix. Figure 2 is a typical plot of $\Delta_n(t)$ for a single initial state, and the average $\langle\Delta(t)\rangle$ over 75 initial states, showing that the evolution is diffusive. Table I shows the diffusion constants obtained by fitting a straight line to the averaged data, together with relevant comparisons with the theory. The error in these estimates for the diffusion constant is approximately $\pm 10\%$. Finally, Fig. 3 is a log-log plot of the scaling function $f_2(\kappa)$, showing good agreement with the asymptotic behavior predicted in Sec. III for small and large κ.

V. DISCUSSION

The results described above give strong evidence for the validity of the theoretical predictions discussed in

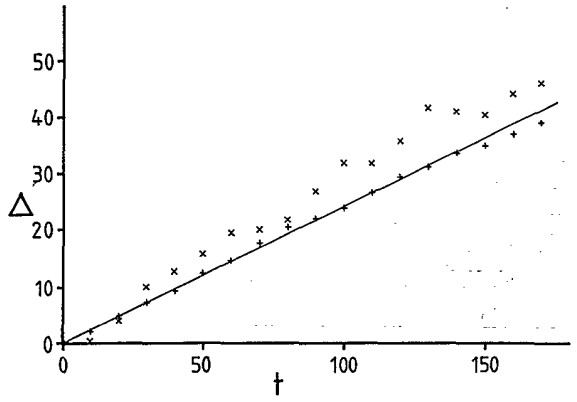

FIG. 2. The time dependence of the second moment $\Delta(t)$ of the occupation probability, for a single state $n=23$ (X) and averaged over 75 states (+), for the GOE model with $N=45$ and $\dot{X}=0.05$. The straight line is a fit to the averaged data, used to estimate the diffusion constant.

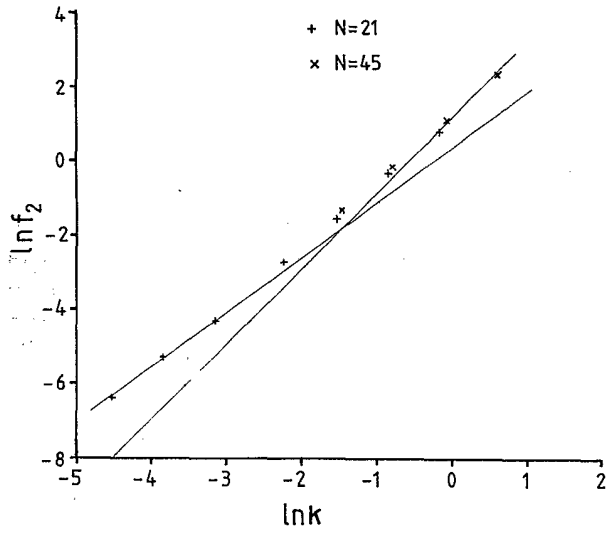

FIG. 3. Graph of $\ln[f_2(\kappa)]$ vs $\ln\kappa$, showing the crossover between the two asymptotic regimes of the diffusion constant described by (3.6) and (3.8), corresponding to the two solid lines with slopes 1.5 (small κ) and 2 (large κ).

Sec. III. In this section we will discuss some limitations on the validity of the theory which apply in some cases where the parameters of the Hamiltonian only explore a finite region.

In the $\kappa \ll 1$ regime, where Landau-Zener transitions are the mechanism of diffusion of the occupation probability, the diffusion can be severely inhibited if there is never a sufficiently narrow gap between two successive energy levels: if the smallest gap ΔE between two energy levels satisfies $\Delta E^2 \gg \hbar\sigma\dot{X}$, then (3.4) implies that the rate of diffusion across this gap will be very small. In the model used for the numerical experiment described above, the coordinate X increases indefinitely, and no matter how small $\dot{X}$ is there will eventually be an avoided crossing with a sufficiently small gap for significant transfer of occupation probability to occur. The size of the smallest gap may, however, be an important consideration if the coordinate X explores a finite region; for instance, if $X(t)$ has a finite amplitude of oscillation, then there will be a finite closest approach between each pair of levels, and the diffusion will be inhibited for sufficiently small values of $\dot{X}$.

If the Hamitonian has several parameters, represented by a vector $\mathbf{X}(t)$, rather than a single parameter $X(t)$, then the evolution of the occupation probability can show true diffusive behavior for arbitrarily small $\dot{\mathbf{X}}$, depending on the dimensionality of the region explored by $\mathbf{X}(t)$. If the vector $\mathbf{X}(t)$ fills a d-dimensional region in the parameter space of the Hamitonian, then the point $\mathbf{X}(t)$ will pass arbitrarily close to points where pairs of energy levels become degenerate if the codimension of these degenerate points is less than or equal to d. A simple argument[3] shows that the codimension of degeneracies in a system with time-reversal invariance and no additional symmetries (such as the GOE) is 2, and for systems without time-reversal invariance (such as the GUE) the codimension is 3. (The codimension of a degeneracy is

TABLE I. Estimates of the diffusion constant $R=\rho^2 D$ for the random matrix model, for various values of the speed parameter $\dot{X}$ and dimension N. The diffusion constants were estimated by calculating $\langle\Delta(t)\rangle$ up to a maximum time $t_{\max}$. Also tabulated are the adiabaticity parameter κ and the scaling function f_2, which is compared with theoretical values for the small κ and large κ asymptotic limits $f_2(\kappa\ll 1)$ and $f_2(\kappa\gg 1)$ calculated from (3.6) and (3.8), respectively.

N	$\dot{X}$	$t_{\max}$	$R=\rho^2 D$	κ	f_2	$f_2(\kappa\ll 1)$	$f_2(\kappa\gg 1)$
21	0.005	3000.0	0.001 15	0.0106	0.001 68	0.001 79	
21	0.01	1000.0	0.003 44	0.0213	0.005 02	0.005 02	
21	0.02	250.0	0.009 10	0.0426	0.0133	0.0142	
21	0.05	80.0	0.0458	0.106	0.0668	0.0562	
21	0.1	30.0	0.141	0.213	0.205	0.159	0.142
21	0.2	12.5	0.476	0.426	0.694		0.569
21	0.4	4.0	1.42	0.851	2.08		2.28
45	0.05	150.0	0.124	0.228	0.265	0.176	0.163
45	0.1	40.0	0.391	0.456	0.835		0.653
45	0.2	12.0	1.35	0.912	2.88		2.61
45	0.4	3.0	4.64	1.82	9.91		10.45

the number of parameters of the Hamiltonian which must be varied in order to force two levels to become degenerate.) If $\mathbf{X}(t)$ passes arbitrarily close to degenerate points, then the corresponding avoided crossings can have an arbitrarily small gap, and diffusion occurs for arbitrarily small velocities $\dot{\mathbf{X}}$ if the dimensionality $d \geq 2$ in the GOE case, or $d \geq 3$ in the GUE case.

Another special case has been discussed by Gefen and Thouless,[9] who considered a time-dependent magnetic flux threaded though a one-dimensional conducting loop, in the limit where the flux varies very slowly, so that Landau-Zener transitions are the mechanism for the transfer of probability. They show that there is a localization of the occupation probability in the energy space which is analogous to the spatial localization of the wave function in the one-dimensional Anderson model, resulting in the system being unable to absorb more than a given amount of energy. The argument leading to this result depends crucially on the fact that the Hamiltonian is periodic in time, so that localization of the eigenfunctions of the evolution operator for one period of the motion (the Floquet operator) implies that there is no diffusion of the occupation probability on long-time scales. Further work is in progress to determine whether the eigenfunctions of the Floquet operator are also localized in the adiabatic representation for more general time-periodic systems.

ACKNOWLEDGMENTS

I am grateful to the Nuffield Foundation for providing a research grant for computing facitilies, and for the hospitality of Dr. W. Swiatecki and his colleagues at the Lawrence Berkeley Laboratory, where much of this paper was written.

APPENDIX A

In this appendix it will be shown that the Pauli exclusion principle does not inhibit the one-body mechanism form dissipation described in Sec. II. This material is included because, even though it is an elementary calculation, the result is apparently not well known.

Without loss of generality we take the initial state of the N fermion system to be a Slater determinant of orthonormal single fermion states

$$\langle x_1, x_2, \ldots, x_N | \Psi_N \rangle = \frac{1}{\sqrt{N!}} \sum_P (-1)^p \psi(x_{P(1)}) \psi(x_{P(2)}) \cdots \psi(x_{P(N)}) , \tag{A1}$$

where the $P(i)$ are the $N!$ possible permutations of the integers $i = 1, \ldots, N$, and p is the parity of the permutation. The Hamiltonian $\hat{H}_N(t)$ is a sum of N equivalent terms, each of which acts only on one particle,

$$\hat{H}_N(t) = \sum_{i=1}^{N} \hat{H}_i(t) . \tag{A2}$$

The evolution operator is a product of the single-particle evolution operators

$$\hat{U}_N(t) = \prod_{j=1}^{N} \hat{U}_j(t), \quad \hat{U}_j(t) = \exp\left[\frac{i}{\hbar} \int_0^t dt' \hat{H}_j(t') \right] , \tag{A3}$$

and after time t the single-particle states ψ_i are transformed into a new orthogonal set ψ_i',

$$|\psi_i'(x_j)\rangle = \hat{U}_j(t) |\psi_i(x_j)\rangle, \quad \langle \psi_i'(x) | \psi_j'(x) \rangle = \delta_{ij} . \tag{A4}$$

Using the above results the expectation value of the energy of the N-particle system can be calculated,

$$E_N(t) = \langle \Psi_N(t) | \hat{H}_N(t) | \Psi_N(t) \rangle = \frac{1}{N!} \sum_P \sum_{P'} (-1)^{p+p'} \sum_{i=1}^{N} \langle \psi_1'(x_{P(1)}) \psi_2'(x_{P(2)}) \cdots \psi_N'(x_{P(N)}) \times | \hat{H}_i | \psi_1'(x_{P(1)}) \psi_2'(x_{P(2)}) \cdots \psi_N'(x_{P(N)}) \rangle . \tag{A5}$$

All the terms vanish except those with $P = P'$, because of the orthogonality of the single-particle states (A4). Using the fact that each term in the Hamiltonian only acts on one particle, the remaining terms can be simplified

$$E_N(t) = \frac{1}{N!} \sum_P \sum_{i=1}^{N} \langle \psi_i'(x_{P(i)}) | \hat{H}_{P(i)}(t) | \psi_i'(x_{P(i)}) \rangle = \sum_{i=1}^{N} \langle \psi_i'(x) | \hat{H}(t) | \psi_i'(x) \rangle , \tag{A6}$$

i.e., the expectation value of the energy of the N-particle system is the sum of the expectation values of the energies of the N independently evolving single-particle states, so that the Pauli exclusion principle does not result in any inhibition of the diffusion of the distribution function. The exclusion principle does of course inhibit two-body scattering at low temperatures, which justifies using an independent quasiparticle approximation in many-body systems.[10]

APPENDIX B

This appendix describes some statistical properties of the matrix elements

$$\left[\frac{\partial H}{\partial X} \right]_{nm} = \left\langle n \left| \frac{\partial \hat{H}}{\partial X} \right| m \right\rangle , \tag{B1}$$

where $|n\rangle, |m\rangle$ are eigenstates of the Hamiltonian $\hat{H}(X)$. The arguments are similar to those used to motivate the definitions of the GOE and GUE random matrix ensembles,[2] but here are concerned with the statistical properties of a given large matrix, rather than with defining an

ensemble with given invariance properties.

We assume that the matrix elements of $\hat{H}$ and $\partial\hat{H}/\partial X$ are available in some discrete basis set whose typical elements will be denoted by primed indices, e.g., $|i'\rangle, |j'\rangle$. The matrix elements $(\partial\hat{H}/\partial X)_{nm}$ are given by a unitary transformation of the matrix elements in the $|i'\rangle, |j'\rangle$ basis,

$$\left[\frac{\partial H}{\partial X}\right]_{nm} = \sum_{i',j'} \langle n|i'\rangle \left\langle i' \left| \frac{\partial \hat{H}}{\partial X} \right| j' \right\rangle \langle j'|m\rangle = \sum_{i',j'} U_{ni'} \left[\frac{\partial H}{\partial X}\right]'_{ij} U^*_{j'm} , \tag{B2}$$

where $U_{ni'} = \langle n|i'\rangle$ are the coefficients of a unitary matrix. If the Hamiltonian is time-reversal invariant, the matrix elements of $\hat{H}$ and $\partial\hat{H}/\partial X$ can be made real, so that the matrix $O_{ni'} = \langle n|i'\rangle$ defining the transformation to the eigenbasis of $\hat{H}$ is orthogonal. If the Hamiltonian $\hat{H}$ has no symmetries or conserved quantities, the matrix elements U_{ni} or O_{ni} of the transformation which diagonalizes $\hat{H}$ is expected to be very complicated, and to have statistical properties which are almost indistinguishable from those of a randomly chosen unitary or orthogonal transformation, satisfying certain constraints. If the basis $|i'\rangle, \ldots, |j'\rangle, \ldots,$ is a natural basis for $\hat{H}$ (e.g., the eigenstates of some other Hamiltonian closely related to $\hat{H}$), then the coefficients $O_{ni'}$ are small when $|n-i|$ is large. The constraint that the $O_{ni'}$ define an orthogonal transformation is

$$\sum_{i'} O_{ni'} O_{i'm} = \delta_{nm} , \tag{B3}$$

which is a sum rule involving many matrix elements. Provided we consider only statistical properties involving a small number of matrix elements we can ignore this constraint and regard the $O_{ni'}$ as independent random variables. These variables have a mean value of zero, and their variance is given by

$$\langle O_{ij} O_{kl}\rangle = \delta_{ik}\delta_{jl} f_{ij} , \tag{B4}$$

where the brackets denote a local average over matrix elements, in the sense described in Sec. III, and $f_{ij} = f_{ji} = f(i,j)$ is small for $|i-j|$ large, and satisfies

$$\sum_j f_{ij} = 1 \tag{B5}$$

in order for this model to be consistent with (B3).

Now we can use this random matrix model for the O_{ni} to calculate the statistical properties of the matrix elements $(\partial H/\partial X)_{nm}$. In the following computations, summation over repeated indices is implied. The mean value of these matrix elements is

$$\left\langle \left[\frac{\partial H}{\partial X}\right]_{nm} \right\rangle = \left\langle O_{ni} \left[\frac{\partial H}{\partial X}\right]'_{ij} O_{mj} \right\rangle = \left[\frac{\partial H}{\partial X}\right]'_{ij} \langle O_{ni} O_{mj}\rangle = \left[\frac{\partial H}{\partial X}\right]'_{ij} \delta_{nm}\delta_i\delta_{ij} f_{ni} = \delta_{nm} f_{ni} \left[\frac{\partial H}{\partial X}\right]'_{ii} = \delta_{nm} \left\langle \left[\frac{\partial H}{\partial X}\right]'_{ii} \right\rangle . \tag{B6}$$

The mean value of the off-diagonal matrix elements is therefore zero, and the mean value of the diagonal matrix elements is the same as a local average of the diagonal elements of $(\partial H/\partial X)'_{ij}$ with a weighting function f. The second moment of these matrix elements is

$$\begin{aligned}
\left\langle \left[\frac{\partial H}{\partial X}\right]^2_{nm} \right\rangle &= \left\langle O_{ni} \left[\frac{\partial H}{\partial X}\right]'_{ij} O_{mj} O_{nk} \left[\frac{\partial H}{\partial X}\right]'_{kl} O_{ml} \right\rangle \\
&= \left[\frac{\partial H}{\partial X}\right]'_{ij} \left[\frac{\partial H}{\partial X}\right]'_{kl} \langle O_{ni} O_{mj} O_{nk} O_{ml}\rangle \\
&= \left[\frac{\partial H}{\partial X}\right]'_{ij} \left[\frac{\partial H}{\partial X}\right]'_{kl} [\langle O_{ni}O_{mj}\rangle\langle O_{nk}O_{ml}\rangle + \langle O_{ni}O_{nk}\rangle\langle O_{mj}O_{ml}\rangle + \langle O_{ni}O_{ml}\rangle\langle O_{mj}O_{nk}\rangle] \\
&= \left[\frac{\partial H}{\partial X}\right]'_{ij} \left[\frac{\partial H}{\partial X}\right]'_{kl} [\delta_{nm}\delta_{ij}\delta_{kl} f_{ni} f_{nk} + \delta_{ik}\delta_{jl} f_{ni} f_{mj} + \delta_{nm}\delta_{il}\delta_{jk} f_{ni} f_{mj}] \\
&= (1+\delta_{nm}) \left[f_{ni} f_{mj} \left[\frac{\partial H}{\partial X}\right]'^2_{ij} \right] + \delta_{nm} \left[f_{ni} \left[\frac{\partial H}{\partial X}\right]'_{ii} \right]^2 \\
&= (1+\delta_{nm}) \left\langle \left[\frac{\partial H}{\partial X}\right]'^2_{ij} \right\rangle + \delta_{nm} \left\langle \left[\frac{\partial H}{\partial X}\right]'_{ii} \right\rangle^2 ,
\end{aligned} \tag{B7}$$

so that the variance of the diagonal matrix elements is twice that of the off-diagonal ones, as claimed in Sec. III.

If the matrix which diagonalizes $\hat{H}$ is unitary, with elements $U_{ni'}$, rather than orthogonal, then (B4) must be replaced by

$$\begin{aligned}
\langle U_{ij} U^*_{kl}\rangle &= \delta_{ik}\delta_{jl} f_{ij} , \\
\langle U_{ij} U_{kl}\rangle &= 0 ,
\end{aligned} \tag{B8}$$

and one of the three terms in (B7) vanishes, so that in this

case the variance of the diagonal matrix elements is equal to that of the off-diagonal elements,

$$\left\langle \left| \left[\frac{\partial H}{\partial X} \right]_{nm} \right|^2 \right\rangle = \left\langle \left| \left[\frac{\partial H}{\partial X} \right]'_{ij} \right|^2 \right\rangle + \delta_{nm} \left\langle \left[\frac{\partial H}{\partial X} \right]'^2_{ii} \right\rangle . \quad \text{(B9)}$$

Finally, we note that the probability distribution of the matrix elements $\langle n|\partial\hat{H}/\partial X|m\rangle$ is Gaussian; this follows from the fact that they are a sum [given by Eq. (B2)] of a large number of terms which are assumed to be independent.

[1]M. Wilkinson, J. Phys. A **21**, 4021 (1988).
[2]*Statistical Theories of Spectra: Fluctuations,* edited by C. E. Porter (Academic, New York, 1965).
[3]M. V. Berry, in *Chaotic Dynamics of Deterministic Systems,* Les Houches Lectures XXXVI, edited by R. Stora and G. Iooss (North-Holland, Amsterdam, 1981).
[4]A. O. Caldeira and A. J. Leggett, Ann. Phys. (N.Y.) **149**, 374 (1983).
[5]D. Bohm, *Quantum Theory* (Prentice-Hall, New York, 1951).
[6]C. E. Zener, Proc. R. Soc. London Ser. A **137**, 696 (1932).
[7]R. Kubo, Can. J. Phys. **34**, 1274 (1956).
[8]D. A. Greenwood, Proc. Phys. Soc. London, Sect. A **68**, 585 (1957).
[9]Y. Gefen and D. J. Thouless, Phys. Rev. Lett. **59**, 1752 (1987).
[10]D. Pines and P. Nozieres, *The Theory of Quantum Liquids I* (Benjamin, Menlo Park, 1966).