

# Chaos and Energy Spreading for Time-Dependent Hamiltonians, and the various Regimes in the Theory of Quantum Dissipation

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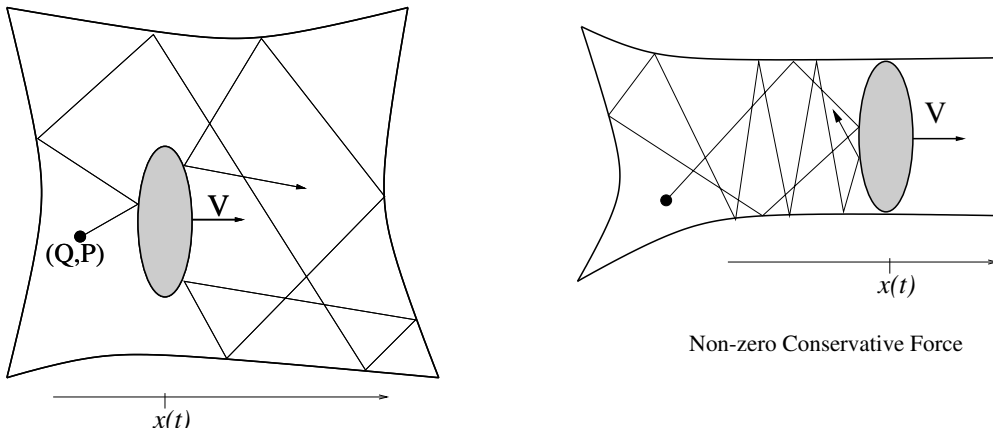
Doron Cohen  
*Department of Physics, Harvard University.*

**Abstract.** We make the first steps towards a generic theory for energy spreading and quantum dissipation. The *Wall formula* for the calculation of friction in nuclear physics and the *Drude formula* for the calculation of conductivity in mesoscopic physics can be regarded as two special results of the general formulation. We assume a time-dependent Hamiltonian  $H(Q, P; x(t))$  with  $x(t) = Vt$ , where  $V$  is slow in a classical sense. The rate-of-change  $V$  is not necessarily slow in the quantum-mechanical sense. The dynamical variables  $(Q, P)$  may represent some ‘bath’ which is being parametrically driven by  $x$ . This ‘bath’ may consist of just few degrees-of-freedom, but it is assumed to be classically chaotic. In case of either the Wall or Drude formula, the dynamical variables  $(Q, P)$  may represent a single particle. In any case, dissipation means an irreversible systematic growth of the (average) energy. It is associated with the stochastic spreading of energy across levels. The latter can be characterized by a transition probability kernel  $P_t(n|m)$  where  $n$  and  $m$  are level indices. This kernel is the main object of the present study. In the classical limit, due to the (assumed) chaotic nature of the dynamics, the second moment of  $P_t(n|m)$  exhibits a crossover from ballistic to diffusive behavior. In order to capture this crossover within quantum-mechanics, a proper theory for the quantal  $P_t(n|m)$  should be constructed. We define the  $V$  regimes where either perturbation theory or semiclassical considerations are applicable in order to establish this crossover. In the limit  $\hbar \rightarrow 0$  perturbation theory does not apply but semiclassical considerations can be used in order to argue that there is detailed correspondence, during the crossover time, between the quantal and the classical  $P_t(n|m)$ . In the perturbative regime there is a lack of such correspondence. Namely,  $P_t(n|m)$  is characterized by a perturbative core-tail structure that persists during the crossover time. In spite of this lack of (detailed) correspondence there may be still a restricted correspondence as far as the second-moment is concerned. Such restricted correspondence is essential in order to establish the universal fluctuation-dissipation relation.

## 1. Introduction

### 1.1. Definition of the problem

We consider in this paper a system that is described by an Hamiltonian  $\mathcal{H}(Q, P; x)$  where  $(Q, P)$  are canonical variables and  $x$  is a parameter. It is assumed that  $\mathcal{H}(Q, P; x)$  with  $x = \text{const}$  generates classically chaotic motion. We are mainly interested in the case of time dependent  $x(t)$ . However, it is assumed that  $\dot{x} = V$  is a classically small velocity. The notion of classical slowness will be defined in Sec.3. The theory that we are going to present is quite general. In some particular applications  $x(t)$  may represent, for example, a time-dependent electric field. However, the theory is best illustrated by considering the ‘piston’ example: In this example  $x$  represent the position of a small rigid body that is translated inside a large cavity, and  $(Q, P)$  are the coordinates of a tiny gas particle. See Fig.1.



**Figure 1.** The ‘piston’ example: The slow degree of freedom is the ‘piston’, and the ‘bath’ consists of one gas particle. In this paper the position of the ‘piston’  $x(t) = Vt$  is treated as a classical parameter. Dissipation means a systematic growth of the bath-energy. For simplicity we assume throughout the paper that the conservative work is zero. This is not the case in the right illustration.

It is assumed that initially the system is characterized by some energy distribution  $\rho(E)$ . In particular we may assume a microcanonical preparation. For  $V = 0$  energy is a constant of the motion, and therefore the energy distribution  $\rho(E)$  will not change as a function of time. On the other hand, for  $V \neq 0$  the energy will be re-distributed and  $\rho(E)$  will become time dependent. In this paper we are interested in the study of this time dependence. Of particular interest is the time dependence of the *first* and of the *second* moments. A systematic increase of the *average* energy has, by definition, the meaning of dissipation. In case of the ‘piston’ example, dissipation means that the gas particle is being ‘heated up’.

### 1.2. Restrictive sense of ‘Quantum dissipation’

The subject of this paper is the quantum-mechanical (QM) theory of energy-spreading and dissipation, as defined in the previous subsection. In short we may say that we are interested in the theory of *Quantum Dissipation*. However, it is important to realize that we are using the term ‘Quantum Dissipation’ in a quite *restrictive sense*. This is because of mainly two reasons: (a) We assume a classical driving force; (b) We are not considering a many-body bath. Note that an infinite number of degrees-of-freedom is not important for having stochastic behavior: this is the main idea behind the term ‘chaos’ when applied to dynamical systems. We can have dissipation even if  $(Q, P)$  represent a few degrees-of-freedom ‘bath’.

The interest in Quantum Dissipation is very old [1, 2, 3, 4, 5, 6, 7]. However, in most of the literature, the term ‘Quantum Dissipation’ is used in a more *general sense*. Namely,  $x$  becomes a dynamical variable, and one looks for its reduced dynamics. Thus, in most of the literature, dissipation-of-energy becomes only one aspect of a much more complicated problem. The ‘grand problem’ includes, besides ‘dissipation’, other issues such as ‘dephasing’ and ‘thermalization’. It also should be noticed that the standard literature usually adopts an effective-bath approach (see subsection 1.4) or other effective formulations [3] that do not necessarily reflect the actual dynamics of the bath degrees-of-freedom. Important exceptions are works such as [31] and [32].

Of particular interest is the ‘piston’ model. If the ‘piston’ is treated as a dynamical object, than its reduced dynamics is called ‘quantal Brownian motion’ (QBM).

According to our (restricted) definition, ‘dissipation’ means systematic irreversible growth of the bath-energy. In case of an un-driven Brownian particle, the ‘dissipation’ is balanced eventually by ‘noise’ leading to ‘thermalization’. In the QM case the issue of ‘irreversibility’ is more complicated because we may have ‘recurrences’. The relevant time scale for these recurrences is the Heisenberg time for the combined BrownianParticle-GasParticle system. This latter time scale may be extremely large if the Brownian particle has a large mass.

In this paper  $x$  is not a dynamical degree of freedom, and therefore the ‘recurrences’ that have been mentioned in the previous paragraph are not an issue. (It is as if we assume that the ‘piston’ has an infinite mass, hence the frequent use of the term ‘moving walls’). For  $V = 0$  the Hamiltonian is time-independent, and we will have recurrences that are associated with the dynamics of the GasParticle (alone). The remnant of this latter type of recurrences is QM-adiabaticity, which we are going to discuss soon. Another type of ‘recurrences’ are associated with *periodic* driving and are discussed in Sec.8. It should become clear from the above discussion, and subsection 1.6 below, that ‘recurrences’ are not an important issue in this paper.

### 1.3. The classical theory of dissipation

The classical understanding of the dissipation-process is based mainly on the works of [4, 5, 8, 9, 11] and followers. We are going to sketch briefly the main idea of the classical theory, and the associated derivation of the fluctuation-dissipation ( $\mathcal{FD}$ ) relation. In the *time-independent case* ( $V = 0$ ) the motion of  $(Q(t), P(t))$  is irregular due to the chaotic nature of the dynamics. We shall denote the ergodic time by  $t_{\text{erg}}$ . We can define a fluctuating quantity  $\mathcal{F}(t) = -(\partial\mathcal{H}/\partial x)$  that has stochastic features. The intensity of these fluctuations will be denoted by  $\nu$ . In the classical case  $\mathcal{F}(t)$  is essentially like noise whose correlation time  $\tau_{\text{cl}}$  is smaller than or equal to  $t_{\text{erg}}$ . In the *time-dependent case* ( $V \neq 0$ ) energy is not a constant of the motion and consequently the energy distribution  $\rho(E)$  becomes time dependent. It is argued that for  $t \gg t_{\text{erg}}$  the energy distribution satisfy a diffusion equation. The energy-dependent diffusion coefficient will be denoted by  $D_{\text{E}}$ . It turns out that quite generally  $D_{\text{E}} = \frac{1}{2}\nu V^2$ . Associated with this diffusion is a systematic growth of the average energy. This systematic growth of energy is due to the  $E$ -dependence of the diffusion process. The rate of energy growth will be denoted by  $\dot{Q}$ . It can be written as  $\dot{Q} = \mu V^2$ .

The considerations above lead to the conclusion that in the classical case the dissipation is of ohmic nature ( $\dot{Q} \propto V^2$ ). The dissipation coefficient is denoted by  $\mu$ . It is implied that the fluctuating quantity  $\mathcal{F}(t)$  has a non-zero average, namely  $\langle \mathcal{F} \rangle = -\mu V$ . In the ‘piston’ example the latter represents the ‘friction’ force that is experienced by the moving object. The considerations above also imply that *the analysis of dissipation is reduced to the study of energy spreading*. The difficult issue is to establish a stochastic energy spreading with a coefficient  $D_{\text{E}} = \frac{1}{2}\nu V^2$ . Then, the  $\mathcal{FD}$  relation between  $\mu$  and the noise intensity  $\nu$  follows as an immediate consequence. If  $\rho(E)$  is a canonical distribution (which is not necessarily the case) then the  $\mathcal{FD}$  relation reduces to the familiar form  $\mu = \nu/(2k_{\text{B}}T)$  where  $T$  is the temperature.

### 1.4. The effective-bath approach to Quantum Dissipation

The most popular approach to ‘Quantum Dissipation’ is the *effective-bath approach* [1, 2, 6, 7]. When applied to ‘our’ problem (as defined in the first subsection) it means that the chaotic  $(Q, P)$  degrees-of-freedom are replaced by an effective-bath that has the same *spectral-properties*. This may be either harmonic-bath (with infinitely many oscillators) or random-matrix-theory (RMT) bath [30].

**Generic classical parameters**  $(\tau_{\text{cl}}, \nu)$  $\tau_{\text{cl}}$  = classical correlation time. $\nu$  = intensity of fluctuations**Generic quantal parameters**  $(\Delta, b, \sigma, \hbar)$  $\Delta$  = mean level spacing of the eigen-energies  $\{E_n\}$  $b$  = Dimensionless bandwidth of the matrix  $(\partial\mathcal{H}/\partial x)_{nm}$  $\sigma$  = Root-mean-square of in-band matrix elements of  $(\partial\mathcal{H}/\partial x)_{nm}$ **Semiclassical relations**

$$\tau_{\text{cl}} = 2\pi\hbar/(b\Delta)$$

$$\nu = (2\pi\hbar/\Delta) \sigma^2$$

**Linear response theory**

$$D_{\text{E}} = \frac{1}{2}\nu V^2 = (\pi\hbar/\Delta) \sigma^2 V^2$$

**Ohmic dissipation**

$$d\langle\mathcal{H}\rangle/dt = \mu V^2$$

$$\mu = \mathcal{FD}[\nu]$$

**Primary dimensionless parameters**  $(b, v_{\text{PR}})$ 

$$v_{\text{PR}} = (1/\hbar) \sqrt{\nu\tau_{\text{cl}}^3} V = b^{-3/2} (2\pi\hbar/\Delta)^2 (\sigma/\hbar) V$$

**Table 1.** Overview of the common theory for dissipation. Two generic parameters should be specified for the classical theory, while four are required for the QM theory. Note that  $V = \dot{x}$  always appears in the combination  $\nu V^2$  or  $\sigma V$ , and therefore it should not be counted as an additional (independent) parameter. The two classical parameters can be expressed in terms of the QM parameters via semiclassical relations. In the absence of well defined classical limit (as in the case of RMT models) this relations can be regarded as definitions. The so called Kubo-Greenwood result of linear response theory can be obtained using FGR picture, and it coincides with the classical expression. General considerations lead to a fluctuation-dissipation ( $\mathcal{FD}$ ) relation between  $\mu$  and  $\nu$ . An important observation of this paper is that the validity of the linear-response approach is controlled by the dimensionless parameter  $v_{\text{PR}}$ .

It turns out that quantal-classical correspondence (QCC) is a natural consequence of this procedure: The dissipation coefficient  $\mu$  turns out to be the same classically and quantum-mechanically. In order to explain this point let us use the Caldeira-Leggett notations [7]. The distribution of the frequencies of the bath-oscillators is characterized by an ohmic spectral-function  $J(\omega) = \eta\omega$ . The classical analysis leads to a friction force with a coefficient  $\mu = \eta$ , and white noise whose intensity is  $\nu = 2\eta k_{\text{B}}T$ . Using Feynman-Vernon [1] formalism one obtains the same value  $\mu = \eta$  in the QM case. The quantal noise is characterized by an  $\hbar$ -dependent power-spectrum, but the noise intensity  $\nu$  is defined as the  $\omega = 0$  component, and it is still equal to  $2\eta k_{\text{B}}T$ . Hence the classical  $\mathcal{FD}$  relation  $\mu = \nu/(2k_{\text{B}}T)$  holds also in the QM case.

The effective-bath approach will not be adopted in this letter since its applicability is a matter of *conjecture*. In this paper we want to have a direct understanding of quantum-dissipation.

### 1.5. The QM theory of Dissipation

Quantum-mechanics introduces additional energy scales, as well as additional parametric scales into the problem (See Table 2). Consequently there are few  $V$  regimes in the QM theory (See Table 3). The QM-adiabatic regime [9] is quite well understood. We shall discuss this regime only briefly since it is not related to the main concern of this paper. The further distinction between the QM-slow regime and the QM-fast regime is the main issue of this paper.

Let us assume that initially the energy is concentrated in one particular level. For extremely slow velocities ( $v_{LZ} \ll 1$ ) and relatively long time the energy will remain mainly concentrated in the initial level. This is the QM-adiabatic approximation. The term ‘QM-adiabaticity’ is a bit confusing, because it actually does not correspond (in the  $\hbar \rightarrow 0$  limit) to adiabaticity in the classical sense. Maybe a better term would be ‘perturbative localization’. In the QM-adiabatic regime Landau-Zener transitions between neighboring levels constitute the predominant mechanism for energy spreading. This mechanism does not correspond to the classical mechanism of energy-spreading. The QM-adiabatic regime is a genuine quantal regime.

For higher velocities ( $v_{LZ} \gg 1$ ) it is essential to take into account transitions between non-neighboring levels. The contribution of near-neighbor transitions to the energy spreading becomes negligible rather than predominant. An obvious approach for the study of energy spreading would be to adopt a Fermi-golden-rule (FGR) picture. FGR is one possible picture of *perturbation theory*. The same results for  $D_E$  and  $\mu$  can be derived by using other, equivalent formulations of perturbation theory. The most popular variation is known as ‘linear response theory’ or as ‘Kubo-Greenwood formalism’. Whatever version of perturbation theory is being used the standard result is always the same (See Table 1). It should be realized that the standard result is in complete correspondence with the classical result, and it becomes identical with the classical result upon taking the formal limit  $\hbar \rightarrow 0$ .

### 1.6. Specific motivation for the preset study

Reading some of the early literature one gets the impression that quantum dissipation is conceptually well-understood. Specifically, it looks as if the perturbative methods are effective for the purpose of constructing a general theory. However, this is a wrong impression. *A general theory of energy spreading is still lacking, a-fortiori there is no general theory of quantum dissipation.* This point becomes most evident once we read the work by Wilkinson and Austin (W&A) [10]. Their observations constitute the original motivation for the present study [13].

W&A [10] have defined two important dimensionless parameters that are associated with the velocity  $V$ . These are, (using our notations), the scaled velocity  $v_{LZ}$ , and the scaled velocity  $v_{RMT}$ . The QM-adiabatic regime is distinguished by the condition  $v_{LZ} \ll 1$ , where we have the relatively simple picture of spreading due to Landau-Zener transitions. At higher velocities ( $v_{LZ} \gg 1$ ) the QM-adiabatic nature of the dynamics is lost, and the Landau-Zener picture no longer apply. In order to extend the perturbative treatment to such higher velocities W&A have suggested to adopt an innocent-looking RMT assumption. As long as the velocity is sufficiently slow ( $v_{RMT} \ll 1$ , but still  $v_{LZ} \gg 1$ ) a classical-like result for  $D_E$  is obtained. On the other hand, once  $v_{RMT} \gg 1$ , the classical-like expression for  $D_E$  no longer holds. It is modified in such a way that correspondence with the classical result is being lost!

Obviously, W&A have realized that the above conclusion is inconceivable. We will have to understand what is wrong with their innocent-looking RMT assumption. We shall argue that  $v_{RMT} \sim 1$  does not mark a crossover to a non-classical regime. Rather, we shall find out that there is a *different* dimensionless parameter ( $v_{PR}$ ) that

<b>Energy Scales:</b>	
$\Delta$	$\propto \hbar^d =$ mean level spacing of the eigen-energies $\{E_n\}$ .
$\Delta_b$	$= b\Delta = 2\pi\hbar/\tau_{cl} =$ bandwidth of the matrix $(\partial\mathcal{H}/\partial x)_{nm}$
$\Delta_{sc}$	$\propto \hbar^{2/3} =$ semiclassical width of Wigner function.
<b>Parametric scales:</b>	
$\delta x_c^{cl}$	$=$ parametric correlation scale of the $x$ -dependent Hamiltonian
$\delta x_c^{qm}$	$= (\Delta/\sigma) \propto \hbar^{(1+d)/2} =$ The $\delta x$ required to mix neighboring levels.
$\delta x_{prt}$	$= \sqrt{b}(\Delta/\sigma) \propto \hbar =$ The $\delta x$ to mix all the levels within the bandwidth.
$\delta x_{sc}$	$\propto \hbar^{2/3} =$ The $\delta x$ required to get detailed QCC.
<b>Temporal scales:</b>	
$\tau_{cl}$	$=$ Classical correlation time of $\mathcal{F}(t)$ .
$t_{erg}$	$=$ Ergodic time of the classical chaotic motion.
$t_{trc}$	$= \nu/(\mu V)^2 =$ Breaktime of the classical adiabatic approximation.
$\tau_c^{qm}$	$= \delta x_c^{qm}/V =$ The time it takes to mix neighboring levels .
$t_{prt}$	$=$ Ultimate breaktime of the QM perturbation theory.
$t_{sdn}$	$=$ Breaktime of the QM sudden approximation.
$t_H$	$= 2\pi\hbar/\Delta =$ Time needed to resolve individual levels (Heisenberg time).

**Table 2.** Various scales in the theory of energy spreading. The generic  $\hbar$  dependence is indicated in most cases. The parametric scales and the temporal scales are associated with the kernels  $P(n|m)$  and  $P_t(n|m)$  respectively. The determination of  $t_{prt}$  and  $t_{sdn}$  is an important issue of this paper. Their dependence on  $V$  is illustrated in Fig.5. It should be realized that  $\tau_{cl}$  can be defined, from a purely QM point of view, as the time which is required in order to resolve the energy scale  $\Delta_b$ . Similarly  $t_{sdn}$  is defined as the time which is required in order to resolve the spreading profile. The time  $t_{sdn}$  can be either equal or shorter than  $\tau_{cl}$ .

controls the route towards quantal-classical correspondence (QCC).

### 1.7. Main claims of this paper

The purpose of this paper is to describe the time-evolution of the energy spreading in the various velocity regimes (See Table 3). The various ‘scenarios’ are graphically illustrated in Fig.5. The main claims of this paper are implied by this illustration. Disregarding the QM-adiabatic regime we are motivated by the following two questions:

- What is the regime where FGR/RMT picture is valid?
- What is the regime where QCC considerations are valid?

In particular we would like to know whether there is a ‘clash’ between FGR/RMT considerations on the one hand, and QCC considerations on the other hand.

The main object of this paper is the transition probability kernel  $P_t(n|m)$ . The variable  $m$  denotes the initial energy-state of the system, and  $n$  stands for one of the instantaneous energy-states at a later time  $t$ . This kernel is well defined quantum-mechanically as well as classically. The energy distribution  $\rho_t(E)$  can be obtained by operating with the kernel  $P_t(n|m)$  on the initial microcanonical preparation  $\rho_{t=0}(E)$ , and making a simple change of variables  $n \mapsto E$ . An important distinction in this paper is between *restricted* QCC and *detailed* QCC. Detailed QCC implies that the

<b>Classical slowness conditions:</b>	
$V\tau_{\text{cl}} \ll \delta x_{\text{c}}^{\text{cl}}$	Trivial condition
$\tau_{\text{cl}} \ll t_{\text{trc}}$	Non-trivial Condition
<b>Quantal regimes:</b>	
$Vt_{\text{H}} \ll \delta x_{\text{c}}^{\text{qm}}$	QM-adiabaticity (extremely slow velocities)
$V\tau_{\text{cl}} \ll \delta x_{\text{prt}}$	QM-slow velocity (linear response regime)
$V\tau_{\text{cl}} \gg \delta x_{\text{SC}}$	QM-fast velocity (semiclassical regime)
<b>Scaled velocities:</b>	
$v_{\text{SC}} = \sqrt{2D_{\text{E}} \tau_{\text{cl}}} / \Delta_{\text{SC}}$	$= V / (\delta x_{\text{SC}} / \tau_{\text{cl}})$
$v_{\text{PR}} = \sqrt{2D_{\text{E}} \tau_{\text{cl}}} / \Delta_{\text{b}}$	$= V / (\delta x_{\text{prt}} / \tau_{\text{cl}})$
$v_{\text{RMT}} = b^{1/2} v_{\text{PR}} = \tau_{\text{cl}} / \tau_{\text{c}}^{\text{qm}}$	$= V / (\delta x_{\text{c}}^{\text{qm}} / \tau_{\text{cl}})$
$v_{\text{LZ}} = b^{3/2} v_{\text{PR}} = t_{\text{H}} / \tau_{\text{c}}^{\text{qm}}$	$= V / (\delta x_{\text{c}}^{\text{qm}} / t_{\text{H}})$

**Table 3.** Definitions of the various  $V$  regimes in the theory of energy spreading and dissipation. The classical slowness condition is always assumed to be satisfied. In the QM case we distinguish between the regimes of QM-adiabaticity (extremely slow velocities), QM-slow velocities, and QM-fast velocities. Dimensionless (scaled) velocities can be defined in order to distinguish between the various regimes. For reasonably small  $\hbar$  we have  $v_{\text{LZ}} \gg v_{\text{RMT}} \gg v_{\text{PR}} \gg v_{\text{SC}}$ . In the classical limit all of them  $\gg 1$ . The condition  $v_{\text{LZ}} \ll 1$  defines the QM-adiabatic regime. The condition  $v_{\text{PR}} \ll 1$  define the regime of QM-slow velocities. The condition  $v_{\text{SC}} \gg 1$  defines the regime of QM-fast velocities. The parameter  $v_{\text{RMT}}$  has been introduced in [10], and we are going to explain that it determines the limitation of an over-simplified RMT approach.

quantal  $P_t(n|m)$  is similar to the classical  $P_t(n|m)$ . We shall see that detailed QCC can be established in an intermediate time regime provided the velocity  $V$  is large enough. In the absence of detailed QCC we still may have restricted QCC. The latter implies that only the first and the second moments of the corresponding distributions (quantal versus classical) are similar. Restricted QCC is sufficient in order to guarantee QCC as far as the diffusion coefficient  $D_{\text{E}}$  and the dissipation coefficient  $\mu$  are concerned. Our main statements are:

- The FGR picture implies restricted rather than detailed QCC.
- The FGR picture is valid in the regime  $v_{\text{PR}} \ll 1$ .
- Detailed QCC considerations are valid in the regime  $v_{\text{SC}} \gg 1$ .

It should be realized that the FGR picture is not *valid* in the regime  $v_{\text{PR}} \gg 1$ . However, this does not necessarily imply that the standard Kubo-Greenwood result is not *correct* there. On the contrary: In the the limit  $\hbar \rightarrow 0$  we have detailed QCC ( $v_{\text{SC}} \gg 1$ ), and at the same time Kubo-Greenwood result simply coincides with the classical result. Thus we may say that for  $v_{\text{SC}} \gg 1$ , the standard Kubo-Greenwood result is not valid but correct. The distinction between ‘valid’ and ‘correct’ is crucial here: A correct result sometimes follows from using wrong assumptions. In the intermediate regime ( $v_{\text{PR}} \gg 1$  but  $v_{\text{SC}} \ll 1$ ) neither FGR nor QCC consideration apply and we may have qualitatively different results for  $\mu$ . It is suspected [24], but not yet proved in the present context, that some artificial RMT models, that does not possess a well defined classical limit, may exhibit for  $v_{\text{PR}} \gg 1$  a significantly different behavior compared with the expected FGR or classical result. This latter observation is in the spirit of [10], but it is quite different as far as details are concerned.

It is important to understand what is the origin of the FGR picture validity condition  $v_{\text{PR}} \ll 1$ , and why it is different from the condition  $v_{\text{RMT}} \ll 1$  that has been suggested in [10]. Again we assume that initially the energy is concentrated in one particular level. We shall argue that in order to determine  $D_E$  it is important to estimate how many levels are mixed non-perturbatively at the time  $t \sim \tau_{\text{cl}}$ . If the related parametric change  $\delta x = Vt$ , does not mix neighboring levels, then we are on “safe ground” of standard first-order perturbation theory (FOPT), and we can trust completely the FGR picture. Such circumstances are guaranteed by the condition  $v_{\text{RMT}} \ll 1$ . If  $v_{\text{RMT}} \gg 1$  we have a breakdown of the standard FOPT picture, but this does not imply that the FGR picture becomes non-valid. It turns out that the FGR result for transition rate between levels is valid on “large” energy scales, even if there is non-perturbative mixing of levels on “small” energy scales. This is true as long as the “small” scale is much smaller compared with the bandwidth  $\Delta_b$  of first-order transitions. Such circumstances are guaranteed by the condition  $v_{\text{PR}} \ll 1$ .

### 1.8. The ‘piston’ example - The wall formula

We are using throughout this paper the ‘piston’ model of Fig.1 as an illustrative example. It should be noticed that for simplicity of presentation we picture the ‘piston’ as a small moving obstacle whose motion is constrained to be in one space direction. From purely linguistic point of view ‘piston’ implies also hermetic closure along the margins. We do not assume such a closure.

Application of the  $\mathcal{FD}$  relation in order to get an expression for the dissipation coefficient  $\mu$  leads to the ‘wall’ formula. This formula has been originally derived using kinetic considerations [4], and only later using other approaches [5, 11], including the  $\mathcal{FD}$  approach that we are using here.

In the *proper classical limit* (taking  $\hbar \rightarrow 0$ , while all the other parameters are held fixed) the walls of the ‘piston’ always become ‘soft’, meaning that De-Broglie wavelength becomes much smaller than the penetration distance. The hard walls limit (meaning that the penetration distance is taken to be zero, while  $\hbar$  is being kept fixed), is non-generic. It is important to understand the consequences of taking this limit. In the hard wall limit  $(\partial\mathcal{H}/\partial x)_{nm}$  is not a banded matrix, and the (generic) problem of having a non-perturbative regime for  $\hbar \rightarrow 0$  is being avoided. The non-generic features of the hard wall limit are possibly responsible for some prevailing miss-conceptions, and in particular to the *illusion* that perturbative techniques can be used in order to get a *general* theory for ‘quantum dissipation’. This is the reason for the inclusion of a quite detailed discussion of the ‘piston’ example. The consequences of taking the hard-wall limit, as well as other non-generic features of the ‘piston’ example are further discussed in the concluding section and in [14].

### 1.9. The ‘mesoscopic’ example - Drude formula

Another physical examples that can be treated by the general theory of dissipation is taken from the realm of mesoscopic physics. Consider the case where  $x$  is the magnetic flux via a ring. The velocity  $V = \dot{x}$  has then the meaning of electro-motive-force. Let us assume that the ring contains one charged particle ( $Q, P$ ) that performs diffusive motion. Ohmic dissipation ( $\dot{Q} = \mu V^2$ ) means that the charged particle gains kinetic energy, where the dissipation coefficient  $\mu$  is just the conductivity of the ring. Equivalently, having  $\langle \mathcal{F} \rangle = -\mu V$  just means that the drift velocity along the ring is proportional to the electro-motive-force. It is a trivial exercise to get Drude formula from the general  $\mathcal{FD}$  relation. The advantage of this procedure is that the derivation can easily be extended to the case where the motion of the charged particle is chaotic



rather than diffusive. It should be noted that in actual circumstances the charged-particle is an electron, and its (increasing) kinetic energy is eventually transferred to the vibrational modes (phonons) of the ring. The latter process (that leads to Joule heating) is ‘on top’ of the generic dissipation problem that we are going to analyze.

### 1.10. Overview of the paper

This paper divides roughly into three parts. The appendixes (A-J) should be considered an integral component in the reading of the main text. The reason for transforming some of the sections into appendixes was the desire to maintain a simple logical flow. We turn now to give a brief description of the paper. The first part of this paper (**sections 2-7**), in a superficial glance, looks like a review. However, in spite of its textbook style, it is not a review. It gives the necessary introduction for the later QM analysis, and in particular it contains a careful examination of the various assumptions that are involved in the common approaches to the theory of dissipation. (It turns out that a satisfactory presentation is lacking in the existing literature). The main items of the first part are:

- The crossover from ballistic to diffusive energy spreading.
- Precise formulation of the classical slowness conditions.
- Brief description of the derivation of the  $\mathcal{FD}$  relation.
- Critical discussion of the QM linear-response theory.
- Critical discussion of the standard FGR picture.
- The wall formula generalized to arbitrary dimensionality ( $d = 2, 3, \dots$ ).

The second part of this paper (**sections 8-10**) contains the precise formulation of the theory and an overview of the general picture. The main items of the second part are:

- Definitions of the kernels  $P(n|m)$  and  $P_t(n|m)$ .
- The stochastic description of the energy spreading process.
- Restricted QCC versus detailed QCC, and the classical approximation.
- Overview of the dynamical scenarios in the different  $V$  regimes.

The third part of this paper (**sections 11-20**) gives a detailed presentation of perturbation theory and RMT considerations. The main items are:

- The Schroedinger equation in the  $x$ -dependent basis.
- The QM-sudden approximation and parametric evolution.
- The over-simplified RMT picture.
- An improved version of perturbation theory.
- The core-tail structure of the spreading kernel.

The paper is concluded (**section 21**) by pointing out some important questions that have been left open. Some future directions for research are indicated.

### 1.11. The need for a generic theory

Our main interest in this paper is to construct a *generic* theory for energy spreading and quantum dissipation. In particular we want to define the conditions for getting ohmic dissipation, to establish the associated  $\mathcal{FD}$  relation and to explore the validity limits of the QCC principle.

One may wonder what is the practical gain in achieving the above mentioned goals. Is it just a matter of doing ‘mathematics’ properly? A similar type of question is frequently asked with regard to the efforts to re-derive well known RMT results using semiclassical methods. The answer to such questions should be clear: It is not possible to analyze non-generic (or non-universal) features unless one possess a thorough understanding of a generic theory along with its limitations. In the future,

our intention is to analyze circumstances that go beyond these limitations, and to look for genuine QM effects [33].

We are using the term ‘generic’ frequently, and it is now appropriate to define what do we mean by that. The answer is as follows: In order to understand a phenomena (energy spreading and dissipation in the present case) it is a common practice to make the maximum simplifications possible. Then we get a theory with a minimal number of parameters. It turns out that the theory of energy spreading involves the minimal number of *two* dimensionless parameters. We are going to consider any additional (dimensionless) parameter as non-generic. Finally, it should be clear that some of our predictions concerning energy spreading are completely non-trivial. The kernel  $P_t(n|m)$ , as well as its parametric version  $P(n|m)$ , are accessible to numerical studies [15, 16] as well as to real experiments.

## 2. Energy surfaces and eigenstates

We consider a system that is described by an Hamiltonian  $\mathcal{H}(Q, P; x)$  where  $(Q, P)$  are canonical variables and  $x$  is a parameter. The phase space volume that corresponds to a the energy surface  $\mathcal{H}(Q, P; x) = E$  is

$$n = \Omega(E; x) = \int \frac{dQdP}{(2\pi\hbar)^d} \Theta(E - \mathcal{H}(Q, P; x)) \quad (1)$$

where  $d$  is the number of degrees of freedom. Measuring phase-space volume in units of  $(2\pi\hbar)^d$  is insignificant classically, but very convenient upon quantization. The density of phase space cells will be denoted by  $g(E) = \partial_E \Omega(E; x)$ . The energy surface that corresponds to a phase space volume  $n$  will be denoted by  $|n(x)\rangle$  and its energy will be denoted by  $E_n(x)$ . We assume a simple phase space topology such that for given  $n$  and  $x$  corresponds a unique energy surface. Thus

$$|n(x)\rangle = \{(Q, P) | \mathcal{H}(Q, P; x) = E_n(x)\} \quad (2)$$

The microcanonical distribution which is supported by  $|n(x)\rangle$  is

$$\rho_{n,x}(Q, P) = \frac{1}{g(E)} \delta(\mathcal{H}(Q, P; x) - E_n(x)) = \delta(\Omega(\mathcal{H}(Q, P; x)) - n) \quad (3)$$

In the QM case the energy becomes quantized, and the mean level density is related to the classical density of phase space cells. By Weyl law we have:

$$\frac{1}{\Delta} \equiv \overline{\sum_n \delta(E - E_n)} = g(E) \quad (4)$$

Thus, upon quantization, the variable  $n$  becomes a level-index, and  $\rho_{n,x}(Q, P)$  should be interpreted as the Wigner function that corresponds to the eigenstate  $|n(x)\rangle$ . With these definitions we will be able to address the QM theory and the classical theory simultaneously. We shall use from now on an admixture of classical and quantum-mechanical jargon. This should not cause any confusion. The QM discussion however is postponed to later sections. The following discussion is purely classical.

Let us consider a set of *parametrically related* energy surfaces  $|n(x)\rangle$  that enclose the same phase space volume  $n$ . By differentiation of the expression  $\Omega(E(x); x) = n$  with respect to the parameter  $x$  one obtains:

$$\delta E = -F(x)\delta x, \quad F(x) \equiv \left\langle -\frac{\partial \mathcal{H}}{\partial x} \right\rangle_E \quad (5)$$

The angular brackets denote microcanonical average over all the phase space points that satisfy  $\mathcal{H}(Q, P; x) = E$ . Later we shall see that the quantity  $F(x)$  has the meaning of a generalized (conservative) force. Having  $F(x) = 0$  for any  $x$  is equivalent to having  $\Omega(E; x)$  which is independent of  $x$ . Such is the case for a gas particle which is affected by collisions with a small rigid body that is being translated inside a large cavity. We shall refer to the latter example as the ‘piston’ example. See Fig.1 and Sec.7 for more details. In order to simplify notations we shall assume, with almost no loss of generality, that indeed  $\Omega(E; x)$  is independent of  $x$ . It is also useful to define

$$\mathcal{F}(Q, P; x) \equiv \left( -\frac{\partial \mathcal{H}}{\partial x} \right) - \left\langle -\frac{\partial \mathcal{H}}{\partial x} \right\rangle_E \quad (6)$$

We can define a parametric correlation scale  $\delta x_c^{\text{cl}}$  that is associated with the function  $\mathcal{F}(Q, P; x)$ . For the ‘piston’ example (to be discussed in Sec.7) it is just the penetration distance into the ‘piston’ upon collision (the effective ‘thickness’ of the wall). If either  $(Q, P)$  or  $x$  become time-dependent, then  $\mathcal{F}$  becomes a fluctuating quantity. The nature of these fluctuations is discussed in the next section.

### 3. Fluctuations

For a given  $x = x(t)$  and initial conditions  $(Q(0), P(0))$  we may find the time-history  $(Q(t), P(t))$ . We shall also use the notations

$$\begin{aligned}\mathcal{E}(t) &\equiv \mathcal{H}(Q(t), P(t); x(t)) \\ \mathcal{F}(t) &\equiv \mathcal{F}(Q(t), P(t); x(t))\end{aligned}$$

The correlator of the fluctuating force is

$$C(t, \tau) \equiv \langle \mathcal{F}(t) \mathcal{F}(t + \tau) \rangle \quad (7)$$

The angular brackets denote microcanonical average over the initial ( $t=0$ ) phase-space point  $(Q(0), P(0))$ . In the next two paragraphs we are going to discuss the statistical properties of the fluctuating force  $\mathcal{F}(t)$ . First we consider the time independent case ( $x = \text{const}$ ), and then the time dependent case.

If  $x = \text{const}$ , then  $\mathcal{E}(t) = E$  is a constant of the motion, and  $C(t, \tau) \equiv C_E(\tau)$  is independent of  $t$ . It is assumed that the dynamics is *chaotic*, and consequently the the stochastic force looks like white noise. The fluctuations spectrum  $\tilde{C}_E(\omega)$  is defined as the Fourier transform of  $C_E(\tau)$ . The intensity of the fluctuations is characterized by the parameter

$$\nu_E \equiv \int_{-\infty}^{\infty} C_E(\tau) d\tau \equiv \tilde{C}_E(\omega=0) \quad (8)$$

The fluctuations are also characterized by a short correlation time  $\tau_{\text{cl}} = \tilde{C}_E(0)/C_E(0)$ . For generic Hamiltonian system it is natural to identify  $\tau_{\text{cl}}$  with the ergodic time  $t_{\text{erg}}$ . However, in specific applications we may have  $\tau_{\text{cl}} < t_{\text{erg}}$ . For the ‘piston’ example, that will be discussed in Sec.7, the correlation time  $\tau_{\text{cl}}$  is equal to the duration of a collision with the wall, while  $t_{\text{erg}}$  is determined by the ballistic time  $\tau_{\text{bl}}$ .

If  $x$  is time dependent rather than a constant, for example  $x(t) = Vt$ , then for any finite  $V$  and  $0 < t$  the actual distribution of  $(Q(t), P(t))$  is no longer microcanonical. The statistical properties of the fluctuating force  $\mathcal{F}(t)$  are expected to be different from the  $V=0$  case. The average  $\langle \mathcal{F}(t) \rangle$  is no longer expected to be zero. Rather, we shall argue (See (22)) that  $\langle \mathcal{F}(t) \rangle = -\mu V$ , where  $\mu$  is the dissipation coefficient. This implies that the correlator  $C(t, \tau)$  acquires an offset  $(\mu V)^2$ . The offset term can be neglected for a limited time  $t < t_{\text{frc}}$

$$t_{\text{frc}} = \nu/(\mu V)^2 \quad [\text{classical breaktime}], \quad (9)$$

provided  $(\mu V)^2 \ll C_E(0)$ . The latter condition, which is equivalent to having

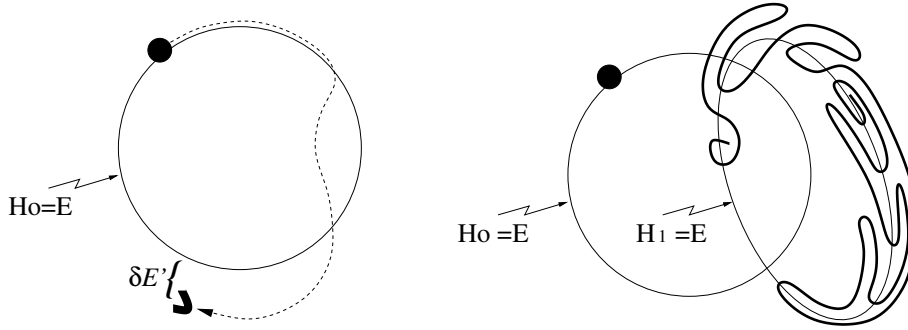
$$\tau_{\text{cl}} \ll t_{\text{frc}} \quad [\text{non-trivial slowness condition}]. \quad (10)$$

implies that the velocity  $V$  should be small enough. There is another possible reason for the correlator  $C(t, \tau)$  to be different from  $C_E(\tau)$ . Loss of correlation may be either due to the dynamics of  $(Q(t), P(t))$  or else due to the parametric change of  $x(t)$ . The correlation time which is associated with the dynamics is  $\tau_{\text{cl}}$ . The correlation time which is associated with the parametric time dependence is  $\tau_c^{\text{cl}} = \delta x_c^{\text{cl}}/V$ . We always assume that

$$\tau_{\text{cl}} \ll \tau_c^{\text{cl}} \quad [\text{trivial slowness condition}]. \quad (11)$$

meaning that loss of correlations is predominantly determined by the chaotic nature of the dynamics rather than by the (slow) parametric change of the Hamiltonian. Since we always assume that that the classical slowness conditions ((10) and (11)) are being satisfied, it follows that we can make the approximation

$$C(t, \tau) = C(\tau) \approx C_E(\tau) \quad \text{for } t < t_{\text{frc}} \quad (12)$$



**Figure 2.** Schematic illustration of the dynamics. An initially localized distribution is launched in phase space. For a limited time (left plot) it travels upon the initial energy surface. But then it departs from it. After much longer times (right plot) the evolving distribution is concentrated across an instantaneous energy surface.

#### 4. Energy spreading and dissipation

For  $x(t) = \text{const}$  the energy  $\mathcal{E}(t)$  is a constant of the motion. For time dependent  $x(t)$  and any particular time-history we can write

$$\frac{d\mathcal{E}}{dt} = \frac{\partial \mathcal{H}}{\partial t} = -(F(x(t)) + \mathcal{F}(t)) \dot{x}$$

The first term implies reversible change of energy due to a conservative force that equals  $F(x)$ . In what follows we shall see that the second term is responsible for an irreversible dissipation process. Integrating over time and using (5) we get

$$\mathcal{E}(t) = E(x(t)) - V \int_0^t \mathcal{F}(t) dt \quad (13)$$

where  $E(x) \equiv E_m(x)$  is the energy that correspond to the initial phase-space volume  $m$ . The difference  $E(x(t)) - E(x(0))$  is due to the reversible work done by the generalized force  $F(x)$ . If we disregard the fluctuating term, then we come to the conclusion that the trajectory is approximately bounded to the evolving energy surface  $|n(x(t))\rangle$ . Thus the phase-space volume  $n = \Omega(\mathcal{E}(t), x(t))$  is an approximate constant of the motion, the so-called ‘adiabatic invariant’. Using (13) we can estimate the energy dispersion which is associated with the fluctuating force:

$$\langle (\mathcal{E}(t) - E(x(t)))^2 \rangle = V^2 \int_0^t dt' \int_{-t'}^{t'} C(t', \tau) d\tau \quad (14)$$

Hence we get a crossover from ballistic to diffusive behavior:

$$\langle (\mathcal{E}(t) - E(x(t)))^2 \rangle \approx C_E(0) \cdot (Vt)^2 \quad \text{for } t \ll \tau_{cl} \quad (15)$$

$$\langle (\mathcal{E}(t) - E(x(t)))^2 \rangle \approx 2D_E t \quad \text{for } \tau_{cl} \ll t \ll t_{frc} \quad (16)$$

The ballistic spreading on short time scales just reflects the parametric change of the energy surfaces. This is the essence of the *sudden approximation* which is illustrated in Fig.2 and further explained in App.Appendix A. The diffusive spreading on longer times reflects the deviation from the *adiabatic approximation*. See illustration in Fig.2 and further details in App.Appendix A. The diffusion coefficient is

$$D_E = \frac{1}{2} V^2 \int_{-t}^t C_E(\tau) d\tau \rightarrow \frac{1}{2} \nu_E V^2 \quad (17)$$

If  $C_E(\tau)$  is short range in nature, then  $D_E$  will tend eventually to the well defined constant value which is indicated in the right hand side of (17). Note that the adiabatic approximation becomes exact in the formal limit  $V \rightarrow 0$ , keeping  $Vt$  constant.

For *intermediate* times  $(Q(t), P(t))$  are distributed ergodically across the evolving energy surface, within a shell of thickness  $\sqrt{2D_E t}$ . We shall argue later (Sec.8) that more generally, for any  $t \gg t_{\text{erg}}$ , the spreading profile  $\rho(E)$  obeys the following diffusion equation

$$\frac{\partial \rho}{\partial t} = \frac{\partial}{\partial E} \left( g(E) D_E \frac{\partial}{\partial E} \left( \frac{1}{g(E)} \rho \right) \right) \quad (18)$$

For simplicity we assume here that there is no conservative work ( $F(x)=0$ ). The energy dependence of the diffusion process implies a systematic growth of the mean energy  $\langle \mathcal{E}(t) \rangle = \int E \rho(E) dE$ . Namely,

$$\dot{Q} \equiv \frac{d}{dt} \langle \mathcal{E} \rangle = - \int_0^\infty dE g(E) D_E \frac{\partial}{\partial E} \left( \frac{\rho(E)}{g(E)} \right) \quad (19)$$

Substituting  $D_E = \frac{1}{2} \nu_E V^2$  and integrating by parts one obtains  $\dot{Q} = \mu V^2$ , along with  $\mathcal{FD}$  relation that can be written schematically as  $\mu = \mathcal{FD}[\nu]$ . The result for  $\mu$  depends on  $\rho(E)$ . If  $\rho(E)$  is well concentrated around some energy  $E$ , one obtains

$$\mu_E = \frac{1}{2} \frac{1}{g(E)} \frac{\partial}{\partial E} (g(E) \nu_E) \quad [\text{microcanonical version}] \quad (20)$$

Another, more familiar variation of the  $\mathcal{FD}$  relation is obtained if one assumes a canonical distribution  $\rho(E) \propto g(E) \exp(-E/(k_B T))$ . By substitution into (19), or simply by canonical averaging over (20), one obtains:

$$\mu_T = \frac{1}{2k_B T} \nu_T \quad [\text{canonical version}] \quad (21)$$

where  $\nu_T$  is related to  $C_T(\tau)$ , and the latter is defined the same way as  $C_E(\tau)$ , but with canonical rather than microcanonical averaging.

Having energy dissipation implies that for  $V \neq 0$  the fluctuating quantity  $\mathcal{F}(t)$  has a non-zero average: From (13), and recalling that we assume  $F(x) = 0$ , we get  $\dot{Q} = \langle \mathcal{F}(t) \rangle V$ . Therefore  $\dot{Q} = \mu V^2$  implies

$$\langle \mathcal{F}(t) \rangle = -\mu V \quad (22)$$

In case of the ‘piston’ example  $V$  is the velocity of the ‘piston’ and  $\langle \mathcal{F}(t) \rangle$  is the associated friction force. In case of conductivity calculation (See Sec.1.9), the parameter  $x$  represents (time-dependent) magnetic flux via a ring,  $V$  is the electro-motive-force, and  $\langle \mathcal{F}(t) \rangle$  is the drift velocity.

## 5. Quantal energy-spreading: Linear response theory

At first sight it seems that the classical derivation in Sec.4 applies also to the QM case provided  $\mathcal{F}(t)$  is treated as an operator. This is essentially the so-called ‘linear response theory’. The only approximation involved is  $C(t, \tau) \approx C_E(\tau)$ . This approximation should be valid as long as the evolving state  $\rho_t(Q, P)$  is similar to the initial *microcanonical preparation*. It is more difficult to satisfy this condition in the QM case. The similarity  $\rho_t(E) \approx \rho_0(E)$  is not a sufficient condition: It is also required that off-diagonal elements of the probability-matrix could be ignored, meaning that a superposition could be treated as if it were an incoherent mixture of the corresponding energy-eigenstates. The classical considerations (Sec.3) lead to the time restriction  $t \ll t_{\text{rec}}$ . The QM considerations will lead to a stronger time restriction  $t \ll t_{\text{prt}}$ . Accordingly, the classical slowness condition (10) is replaced by:

$$\tau_{\text{cl}} \ll t_{\text{prt}} \quad [\text{quantal slowness condition}]. \quad (23)$$

The determination of  $t_{\text{prt}}$ , which is the breake time for QM perturbation theory, will be discussed in later sections. For non-slow velocities, (meaning throughout this paper that (10) and (11) are satisfied but (23) is violated), the following elementary considerations does not apply. The quantal slowness condition (23) should not be confused with the QM-adiabaticity condition (to be discussed later). QM-adiabaticity requires extremely slow velocities.

The QM version of the derivation in Sec.4 gives a classical look-alike result for the energy spreading. The only implicit modification is that the classical  $C_E(\tau)$  should be replaced by the corresponding QM object. For the purpose of concise presentation, the formula for the energy spreading can be written as follows:

$$\delta E^2 = V^2 \int_0^t \int_0^t C_E(t_2 - t_1) dt_1 dt_2 = V^2 t \int_{-\infty}^{+\infty} \frac{d\omega}{2\pi} \tilde{C}_E(\omega) \tilde{F}_t(\omega) \quad (24)$$

where

$$\tilde{F}_t(\omega) = t \cdot (\text{sinc}(\omega t/2))^2 \quad (25)$$

Now  $C_E(\tau)$  is a QM object, and its Fourier transform  $\tilde{C}_E(\omega)$  can be expressed as

$$\tilde{C}_E(\omega) = \sum_n \left| \left( \frac{\partial \mathcal{H}}{\partial x} \right)_{nm} \right|^2 2\pi \delta \left( \omega - \frac{E_n - E_m}{\hbar} \right) \quad (26)$$

One observes that the power-spectrum of the QM fluctuations has a discrete nature, and consequently the correlation function  $C_E(\tau)$  is characterized by the additional time scale  $t_H$ . We assume that  $\hbar$  is reasonably small such that  $\tau_{\text{cl}} \ll t_H$ . Correspondence considerations imply that the quantal  $C_E(\tau)$  is similar to the classical  $C_E(\tau)$  as long as  $t \ll t_H$ . Equivalently, as long as  $t \ll t_H$  the discrete nature of the quantal  $\tilde{C}_E(\omega)$  can be ignored, and we can effectively use the classical  $\tilde{C}_E(\omega)$ . Recall that the power-spectrum of the classical fluctuations looks like that of white noise: It satisfies  $\tilde{C}_E(\omega) \approx \nu_E$  for  $|\omega| \ll 1/\tau_{\text{cl}}$  and decays rapidly to zero outside of this regime. Thus, for  $t \ll \tau_{\text{cl}}$  we can make the replacement  $\tilde{F}_t(\omega) \rightarrow t$ , and we obtain the ballistic result  $\delta E^2 = C_E(0) \cdot (Vt)^2$ , while for  $t \gg \tau_{\text{cl}}$  we can make the replacement  $\tilde{F}_t(\omega) \rightarrow 2\pi\delta(\omega)$ , and we get then the diffusive behavior  $\delta E^2 = \nu_E V^2 t$ .

We can get a semiclassical estimate for the matrix elements in (26) by exploiting the correspondence that has been mentioned above [22]. The function  $\tilde{C}_E(\omega)$  is assumed to be vanishingly small for  $\omega \gg 1/\tau_{\text{cl}}$  which implies that  $(\partial \mathcal{H}/\partial x)_{nm}$  is a banded matrix. Energy levels are coupled by matrix elements provided  $|E_n - E_m| < \Delta_b$  where

$$\Delta_b = \frac{2\pi\hbar}{\tau_{\text{cl}}} = \text{band width} \quad (27)$$

For  $\omega \ll 1/\tau_{\text{cl}}$  the smoothed  $\tilde{C}_E(\omega)$  should be equal to the classical noise intensity  $\nu_E$ . Consequently one obtains the following estimate for individual matrix elements within the band:

$$\sigma^2 = \left| \left( \frac{\partial \mathcal{H}}{\partial x} \right)_{nm} \right|^2 \approx \frac{\Delta}{2\pi\hbar} \nu_E \quad \text{for } |E_n - E_m| < \Delta_b \quad (28)$$

It is important to specify the minimal number of (generic) parameters that are involved in the above analysis. In the classical problem there are just two generic parameters: Namely,  $\tau_{\text{cl}}$  and  $\nu_E$ . Quantum-mechanics requires the specification of *two* additional parameters: Namely, the band width  $\Delta_b$  and the mean level spacing  $\Delta$ . The associated dimensionless parameters are:

$$v_{\text{PR}} = \text{scaled velocity} = \sqrt{2D_E \tau_{\text{cl}}} / \Delta_b \quad (29)$$

$$b = \text{scaled band width} = \Delta_b / \Delta \quad (30)$$

The specification of  $\Delta$  is not dynamically significant as long as  $t \ll t_H$ . Longer times are required in order to resolve individual energy levels. Thus we come to the conclusion that in the time regime  $t \ll t_H$  there is a *single* generic dimensionless parameter, namely  $v_{\text{PR}}$ , that controls QCC. We shall see that the QM definition of slowness (23) can be cast into the form  $v_{\text{PR}} \ll 1$ .

## 6. Quantal energy spreading: The conventional FGR picture

Equation (24) for the QM energy spreading can be derived using linear response theory, i.e. by following the same steps as in Sec.4. However, the simplicity of linear response theory is lost once we try to formulate a controlled version of it. It is difficult to derive and to get a good understanding for the breaktime scale  $t_{\text{prt}}$ . It is better to use the conventional version of time-dependent first-order perturbation theory (FOPT), and to view the energy spreading as arising from *transitions between energy levels*.

The choice of basis for the representation of the dynamics is a crucial step in the analysis. The proper basis for the understanding of energy spreading is the  $x$ -dependent set of eigenstates  $|n(x)\rangle$  of the Hamiltonian  $\mathcal{H}(Q, P; x(t))$ . This is the basis that we are going to use later in this paper. In a sense we are going to introduce an *improved* version of FGR picture. However, for sake of completeness, we would like to discuss in this section the capabilities and the limitations of the *conventional* FGR picture. The conventional FGR picture is using a *fixed basis* that is determined by the unperturbed Hamiltonian  $\mathcal{H}(Q, P; x(0))$ . It should be clear that transitions between unperturbed energy levels reflect reduced-energy-changes rather than actual-energy-changes (see corresponding classical definitions in App.Appendix A). Therefore the description of the crossover from ballistic to diffusive energy spreading is out-of-reach for this version of perturbation theory.

The *conventional* FGR picture can be used in order to determine the diffusion coefficient  $D_E$ , as well as the perturbative breaktime  $\tau_{\text{prt}}$ . A detailed derivation can be found in App.Appendix B). We use the notation  $\tau_{\text{prt}}$  rather than  $t_{\text{prt}}$ , because a different version of perturbation theory is involved here. The final result is  $D_E = \frac{1}{2}\nu_E^{\text{eff}}V^2$ , with the effective noise intensity:

$$\nu_E^{\text{eff}} = \int_{-\infty}^{+\infty} C_E(\tau) F(\tau) S(\tau) d\tau \quad (31)$$

where  $F(\tau)$  is the correlation function of the driving source,  $S(\tau) = \exp(-(\Gamma/2)t)$  is the survival amplitude, and  $\tau_{\text{prt}} = 1/\Gamma$ . The introduction of  $S(\tau)$  is a common ad-hoc improvement of equation (B.3). Such type of improvement is used in other contexts to get the Wigner-Weisskopf Lorentzian line shape. It approximates the effect of higher orders of time-dependent perturbation theory. It is also important to specify the validity condition of the FGR picture. It is not difficult to be convinced that the requirement (B.4) can be relaxed slightly, and the actual condition is:

$$\text{FGR-condition: } \text{Either } \tau_{\text{cl}} \text{ or } \tau_c \ll \tau_{\text{prt}} \quad (32)$$

Here  $\tau_c$  characterizes the correlation function  $F(\tau)$ , namely, it is the correlation time of the driving source. It should be realized that having  $\tau_c \gg \tau_{\text{cl}}$  constitutes an obvious variation of the trivial slowness condition (11). Furthermore, using (B.5) one can easily conclude that a necessary condition for the applicability of FGR picture is  $v_{\text{PR}} \ll 1$ , which coincides with the quantal slowness condition (23). Thus, it is *not possible in principle* to apply the FGR picture in the limit  $\hbar \rightarrow 0$ .

The consistency of the FGR result (31) with the linear response result (24) is not obvious. It is true that (24) gives a crossover from ballistic to diffusive behavior, where indeed  $D_E = \frac{1}{2}\nu_E^{\text{eff}}V^2$ . But if one takes (24) seriously for  $t \gg t_H$ , one will come to the conclusion that this diffusion will stop due to recurrences [12]. The FGR result (31),



due to the presence of  $S(\tau)$ , does not imply such a conclusion, provided  $\tau_{\text{prt}} \ll t_{\text{H}}$ . A vanishingly small result for  $D_{\text{E}}$  is obtained only in the QM-adiabatic regime where we may have  $\tau_{\text{prt}} \gg t_{\text{H}}$ . In the QM-adiabatic regime Landau-Zener transitions between neighboring levels become the predominant mechanism for energy spreading [9], and the FGR picture becomes of minor importance.

## 7. The ‘piston’ example and the wall formula

The above picture and considerations become much more transparent once applied to cavities with moving walls. The Hamiltonian  $\mathcal{H} = E(\mathbf{p}) + \mathcal{V}(\mathbf{x})$  describes the free motion of a ‘gas particle’, whose canonical coordinates are  $Q = \mathbf{x}$  and  $P = \mathbf{p}$ , inside a  $d$ -dimensional space which is confined by some boundary. Unless otherwise specified  $E(\mathbf{p}) = \mathbf{p}^2/2m$  where  $m$  is the mass of the gas particle. The corresponding velocity will be denoted by  $v_{\text{E}}$ . The boundary is composed of wall-elements, and may have few components. For example it may consist of some ‘static’ component that defines an interior space, and an additional ‘moving’ component that defines an excluded space of an impenetrable ‘piston’ as in Fig.1. The displacement of the moving wall-elements is parameterized by  $x$ . The gas particle undergoes elastic collisions with the boundary. The ballistic time will be denoted by  $\tau_{\text{bi}}$ . It is determined by the collision rate with the walls. The derivation in App.Appendix F gives the result:

$$\frac{1}{\tau_{\text{col}}} = \left\langle \sum_{\text{col}} \delta(t - t_{\text{col}}) \right\rangle = \frac{1}{2} \frac{\text{Area}}{\text{Volume}} \langle |\cos \theta| \rangle v_{\text{E}} \quad (33)$$

The  $d$ -dependent geometrical factor  $\langle |\cos \theta| \rangle$  is defined in App.Appendix D. For the purpose of ‘ballistic-time’ definition we should take the total Area of all the wall elements. For the purpose of calculating an effective collision rate the *effective* Area should be defined as in (35). For the ‘piston’ example the total effective Area of the moving-faces of the ‘piston’ may be much smaller compared with the total Area of the walls, and consequently the effective time between collisions will be much larger than the ballistic time.

For the later QM considerations it is essential to consider ‘soft walls’. For concreteness we may assume that the wall is realized by a constant force field  $f$ . If  $z$  is a coordinate perpendicular to a wall elements, than the potential barrier is  $\mathcal{V}(z) = 0$  for  $z < 0$  and  $\mathcal{V}(z) = f \cdot z$  for  $z > 0$  up to some maximal value  $\mathcal{V}_{\text{wall}}$  well inside the barrier. We assume that the energy  $E$  of the particle is much lower than  $\mathcal{V}_{\text{wall}}$ , and therefore the latter energy scale should be of no significance. For strongly chaotic billiards successive collisions with the ‘piston’ are uncorrelated and therefore the classical correlation time  $\tau_{\text{cl}}$  is equal to the collision time with the wall. Namely

$$\tau_{\text{cl}} = (2mv_{\text{E}})/f \quad (34)$$

Obviously, in the hard wall limit  $f \rightarrow \infty$  we have  $\tau_{\text{cl}} \rightarrow 0$ . The displacement of the walls is parameterized by some parameter  $x$ . With each surface-element  $ds$  we can associate a normal unit vector  $\mathbf{n}$ , and a ‘propagation velocity’ which will be denoted by  $\hat{\mathbf{V}}(\mathbf{s})$ . The latter is simply the derivative of the wall-element displacement by the controlling parameter  $x$ . The effective moving-wall area is defined as follows:

$$\text{Area} = \oint (\mathbf{n} \cdot \hat{\mathbf{V}})^2 ds \quad (35)$$

Due to ergodicity there are two different strategies that can be applied in order to calculate  $\nu_{\text{E}}$ . One possibility is to average  $\mathcal{F}(t)\mathcal{F}(t+\tau)$  over  $(\mathbf{x}, \mathbf{p})$ , as implied by the definition (7), and then to integrate over  $\tau$ . Schematically the calculation goes as follows:  $\langle \mathcal{F}^2 \rangle$  simply equal to  $f^2$  multiplied by the ratio between the collision-volume ( $\text{Area} \times (v_{\text{E}}\tau_{\text{cl}})$ ) and the total Volume. Note that the latter ratio simply equals

$\tau_{\text{cl}}/\tau_{\text{col}}$ . The noise intensity is obtained by further multiplication with  $\tau_{\text{cl}}$ . The proper calculation should be done as in App.Appendix E. The other possibility to calculate  $\nu_{\text{E}}$  is to write  $\mathcal{F}(t)$  as a sum over short impulses and to perform the averaging in time domain. The magnitude of the impulses is  $2mv_{\text{E}}$ . The noise intensity is simply equal to the square of the impulses multiplied by the collision rate. The exact calculation is done in App.Appendix F. Both approaches give obviously the same result:

$$\nu_{\text{E}} = 2\langle |\cos\theta|^3 \rangle \frac{\text{Area}}{\text{Volume}} m^2 v_{\text{E}}^3 \quad (36)$$

This result is quite general, but it assumes that successive collisions with the ‘piston’ are uncorrelated. More generally, correlations between successive collisions should be taken into account. The derivation can be done by following an essentially identical computation by Koonin [5] and the result is cast into the form

$$\nu_{\text{E}} = \oint \oint ds_2 ds_1 (\mathbf{n} \cdot \hat{\mathbf{V}}(\mathbf{s}_2)) \nu(\mathbf{s}_2, \mathbf{s}_1) (\mathbf{n} \cdot \hat{\mathbf{V}}(\mathbf{s}_1)) \quad (37)$$

If one ignores correlations between successive collisions, then one obtains  $\nu(\mathbf{s}_2, \mathbf{s}_1) \propto \delta(\mathbf{s}_2 - \mathbf{s}_1)$  and (37) reduces to (36). Using the  $\mathcal{FD}$  relation one obtains the following generalized ‘wall formula’:

$$\mu_{\text{E}} = 2\langle |\cos\theta| \rangle \frac{\text{Area}}{\text{Volume}} m v_{\text{E}} \quad (38)$$

The familiar  $d=3$  version of the wall formula is obtained by substituting  $\langle |\cos(\theta)| \rangle = 1/2$ . As in the case of  $\nu_{\text{E}}$  we can try to derive this result using a simple-minded time-domain approach. See App.Appendix F. It turns out that only *half* of the correct result is obtained. Alternatively, the correct result (38) can be obtained by extending the standard ‘kinetic’ derivation. See App.Appendix G. The kinetic derivation demonstrates that (38) is more general than it seems at first sight. It applies to any velocity-momentum dispersion relation. The mass  $m = (dv/dp)^{-1}$  may be energy dependent.

The QM calculation of  $\nu_{\text{E}}^{\text{eff}}$  requires the knowledge of the quantal  $C_{\text{E}}(\tau)$ , and we should also have a proper understanding of  $F(\tau)$ . For the time being let us assume that the effective  $\tau_{\text{c}}$  is much larger than  $\tau_{\text{cl}}$ . It means that the transitions are resonance-limited, and detailed knowledge of  $F(\tau)$  becomes irrelevant. If the De-Broglie wavelength  $\lambda_{\text{E}} = 2\pi\hbar/(mv_{\text{E}})$  is much smaller compared with other (classical) scales, then it is expected to have QCC, as discussed previously with respect to (26). However, it is also possible to make a direct estimate of the matrix elements that appear in (26). See App.Appendix I. The results are in complete agreement with our semiclassical expectations. Indeed, the bandwidth is determined by the collision time with the (soft) walls (see App.Appendix J), and the power-law decay of matrix elements outside the band can be associated with the discontinuity (see App.Appendix E) in the derivative of the classical  $C_{\text{E}}(\tau)$  at  $\tau = 0$ . The expression for the effective noise intensity can be cast into the form of (37) with

$$\nu(\mathbf{s}_2 - \mathbf{s}_1) = \Omega_d \frac{\text{Area}}{\text{Volume}} m^2 v_{\text{E}}^3 \frac{1}{\lambda_{\text{E}}^{d-1}} \left( \text{Sinc} \left( \frac{2\pi}{\lambda_{\text{E}}} |\mathbf{s}_2 - \mathbf{s}_1| \right) \right)^2 \quad (39)$$

The Sinc function, as well as other notations, are defined in App.Appendix D. The QM result coincides with the classical result if  $\lambda_{\text{E}}$  is small compared with the classical length scales that describe the  $\mathbf{s}$ -dependence of  $\mathbf{n} \cdot \mathbf{V}(\mathbf{s})$ . It is also assumed that  $\lambda_{\text{E}}$  is small compared with the surface radius-of-curvature, else further corrections are required [5].

## 8. The route to stochastic behavior

In this section we shall introduce a general phase-space formulation for the theory of energy-spreading. The main mathematical object of the study, namely the kernel  $P_t(n|m)$ , will be defined. In order to go smoothly from the classical theory to the QM theory it is essential to use proper notations. From now on we use the variable  $n = \Omega(E)$  instead of  $E$ . See definitions in Sec.2. The transition probability kernel  $P_t(n|m)$  is defined as the projection of an evolving state on the instantaneous set of energy-states. It is also possible to define a parametric kernel  $P(n|m)$ . The latter depends on the displacement  $\delta x$  but not on the actual time that it takes to realize this displacement. The definitions are:

$$P_t(n|m) = \text{trace}( \rho_{n,x(t)} \mathcal{U}(t) \rho_{m,x(0)} ) \quad (40)$$

$$P(n|m) = \text{trace}( \rho_{n,x(t)} \rho_{m,x(0)} ) \quad (41)$$

In the above definitions the initial energy-surface is  $|m(x(0))\rangle$ , and the associated phase-space density is  $\rho_{m,x(0)}(Q, P)$ . In the QM-case  $|m(x(0))\rangle$  is an energy-eigenstate and  $\rho_{m,x(0)}(Q, P)$  is the associated Wigner function. The evolving surface/state is represented by  $\mathcal{U}(t) \rho_{m,x(0)}$ , where  $\mathcal{U}(t)$  is either the classical Liouville propagator or its QM version. In the classical case it simply re-positions points in phase-space. In the QM case it propagates a Wigner function and it may have a more complicated structure. The trace operation is just a  $dQdP$  integral over phase-space. In the QM-case the definitions of  $P(n|m)$  and  $P_t(n|m)$  can be cast into a much simpler form using Dirac's notations: See (58) and (59).

In the classical case the kernel  $P(n|m)$  reflects the parametric correlations between two sets of energy surfaces (Fig.3 upper left). Consequently non-Gaussian features may manifest themselves. An important special non-Gaussian feature is encountered in many specific examples where  $x$  affects only a tiny portion of the energy surface. (Fig.3 upper right). In the 'piston' example this is the case because  $(\partial\mathcal{H}/\partial x) = 0$  unless  $Q$  is near the face of the piston. Consequently  $P(n|m)$  will have a  $\delta$ -singularity for  $n = m$ .

The classical scenario for  $P_t(n|m)$  consists of three time regimes. For short times we have the classical *sudden approximation*:

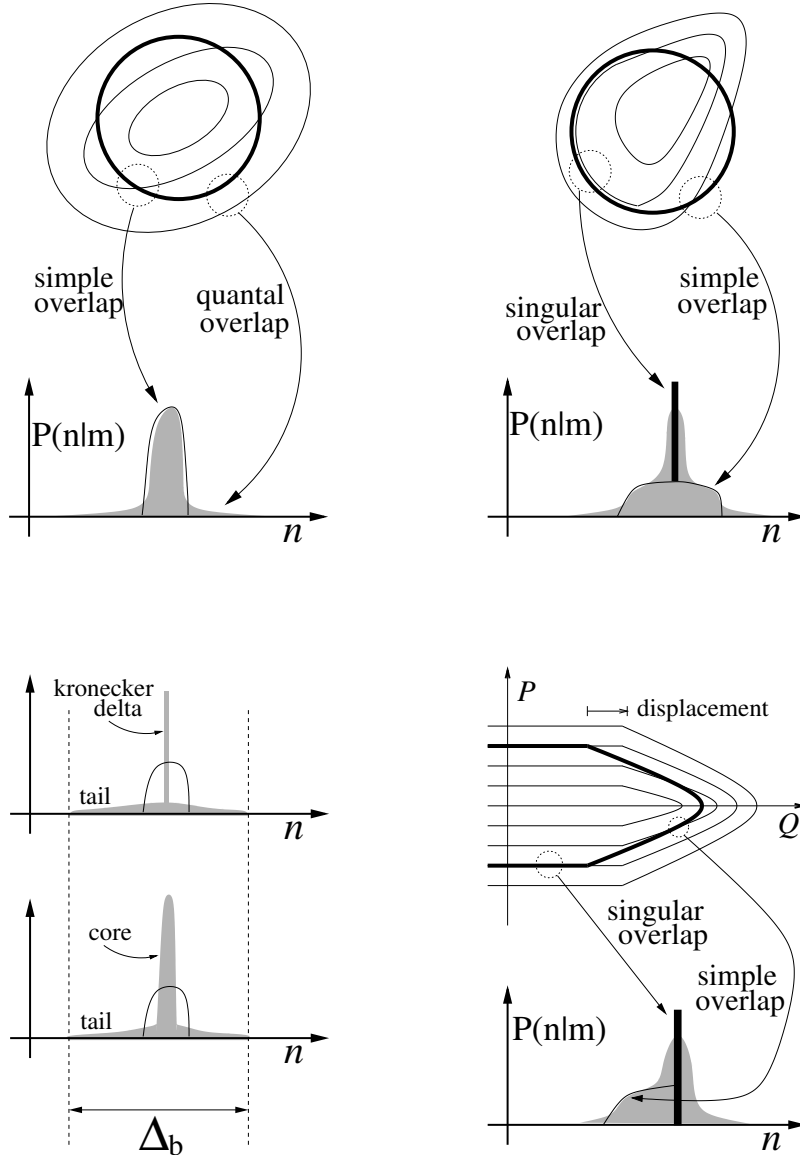
$$P_t(n|m) \approx P(n|m) \quad \text{for } t \ll \tau_{\text{cl}} \quad (42)$$

See Fig.2 and App.Appendix A for more details. For longer times we have the classical *adiabatic approximation*, or more precisely we have diffusive spreading:

$$P_t(n|m) \approx \text{Gaussian}(n-m) \quad \text{for } t_{\text{erg}} \ll t \ll t_{\text{frc}} \quad (43)$$

For  $t \gg t_{\text{frc}}$  the kernel  $P_t(n|m)$  is no-longer a narrow Gaussian that is centered around  $n = m$ . Using (9) it is easily observed that  $t > t_{\text{frc}}$  is equivalent to  $\dot{Q}t > \sqrt{2D_{\text{E}}}t$ , meaning that the systematic energy change becomes larger than the width of the spreading. Thus  $t_{\text{frc}}$  should be regarded as the *brektime* for the classical adiabatic approximation.

On time scales larger than  $t_{\text{erg}}$  one may argue that the energy spreading is like a *stochastic process*, and consequently the diffusive behavior should persist beyond  $t_{\text{frc}}$ . A precise formulation of this point will be presented now. For  $t \gg t_{\text{erg}}$  the evolving surface  $\mathcal{U}(t)|m(x(0))\rangle$  becomes very convoluted due to 'mixing'. As long as one does not insist on looking for fine structures,  $\rho_t(Q, P)$  can be replaced by its smeared version. Any 'tangential' non-homogeneity in phase space will be washed away due to the ergodic behavior, and therefore the smeared  $\rho_t(Q, P)$  is fully characterized by the projected distribution  $\rho_t(n)$ . Obviously this statement is true only if  $t_{\text{erg}}$  is much smaller than the time scale  $t_{\text{frc}}$  that characterizes the 'transverse' spreading. Thus the



**Figure 3.** *Upper Left:* Phase space illustration of the initial and of the instantaneous set of parametric energy surfaces; Plot of the associated  $P(n|m)$ , where the classical behavior is indicated by the black lines, and the QM behavior is represented by the grey filling. Detailed QCC is assumed. In the QM case classical sharp-cutoffs are being smeared. *Upper Right:* Illustration of a typical non-generic feature. In the QM case the classical delta-singularity is being smeared. *Lower Right:* The same non-generic feature manifests itself in the 'piston' example. *Lower Left:* In the perturbative case there is no detailed QCC. The kernel is characterized by a core-tail structure. The tail is limited by the bandwidth of the coupling matrix-elements. If  $\delta x$  is sufficiently small the core is just a kronecker delta.

dynamics acquires the following stochastic property:

$$P_{t_1+t_2}(n|m) \approx \int P_{t_2}(n|n') dn' P_{t_1}(n'|m) \quad \text{provided } t_1, t_2 \gg t_{\text{erg}} \quad (44)$$

Assuming that  $t_{\text{erg}} \ll t_{\text{frc}}$ , it is possible to define an intermediate time  $t_1 = t/N$ , where  $N$  is some large integer, such that  $t_{\text{erg}} \ll t_1 \ll t_{\text{frc}}$ . Using the stochastic property (44) one can write  $P_t(n|m)$  as a convolution of the  $N$  kernels  $P_{t_1}(n|m)$ . Applying the same considerations as in the derivation of the central limit theorem, we come to the conclusion that  $P_t(n|m)$  will become a spreading Gaussian that obeys the diffusion equation

$$\frac{\partial \rho}{\partial t} = \frac{\partial}{\partial n} \left( D_n \frac{\partial \rho}{\partial n} \right) \quad (45)$$

which is equivalent to (18). Note that  $D_n = g(E)^2 D_E$ . This description holds on time scales larger than  $t_{\text{erg}}$ , irrespective of the detailed structure of  $P_{t_1}(n|m)$ . Only the second moment of the latter is important for the determination of the diffusion coefficient.

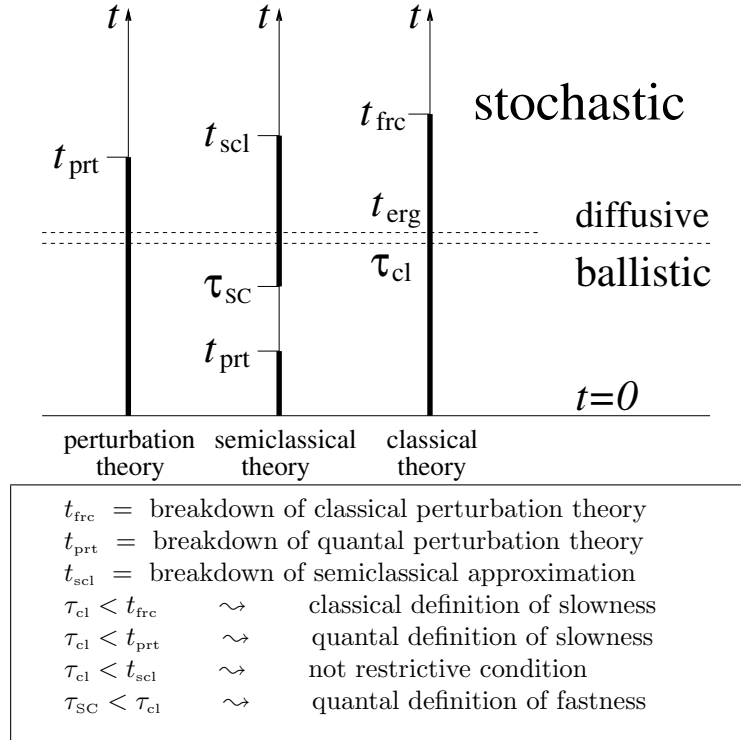
The argumentation in favor of long-time stochastic behavior is more subtle in the QM case. Using obvious notations the stochastic assumption (44) is:

$$\left\langle \left| \langle n | \mathbf{U}_{t_2} \mathbf{U}_{t_1} | m \rangle \right|^2 \right\rangle \approx \sum_{n'} \left\langle \left| \langle n | \mathbf{U}_{t_2} | n' \rangle \right|^2 \right\rangle \left\langle \left| \langle n' | \mathbf{U}_{t_1} | m \rangle \right|^2 \right\rangle \quad (46)$$

Later we shall argue that  $\mathbf{U}$  is a banded matrix. It is true in general that in the absence of correlations between successive unitary operations we will always have a stochastic diffusive behavior [25]. Thus, in order to establish a stochastic behavior in the QM case we should look for a time scale  $\tau_c$  that marks the loss of phase-correlation. For  $t_1, t_2 \gg \tau_c$  we can argue that the off-diagonal 'interference' terms in the matrix multiplication  $\mathbf{U}_{t_2} \mathbf{U}_{t_1}$  will be averaged to zero.

One way to establish the existence of a time scale  $\tau_c$  is just to assume *irregular* driving. As an example let us assume that we have a 'piston' that is pushed back and forth in arbitrary a-periodic fashion, meaning that  $\dot{x}(t)$  becomes uncorrelated on a time scale that will be denoted by  $\tau_c^{\text{drv}}$ . The irregular driving is like noise and consequently the interference contribution is averaged to zero [25]. For *periodic* driving, there may be limitation of diffusion due to 'localization' effect as in the quantum-kicked-rotator model [25]. The study of this latter issue is beyond the scope of this paper. As in the classical case we will be able to establish a diffusive behavior on an *intermediate* time scale. QM considerations will be limited either by a semiclassical breaktime  $t_{\text{scl}}$  or by a perturbative breaktime  $t_{\text{prt}}$ , which are analogous to the classical breaktime  $t_{\text{frc}}$ . If we do not have the separation of time scales ( $\tau_c^{\text{drv}} \ll t_{\text{prt}}$  or  $\tau_c^{\text{drv}} \ll t_{\text{scl}}$ ) then we should wonder whether there is an *intrinsic*  $\tau_c$ . An intrinsic  $\tau_c$  is expected to be either equal or larger than the classical time  $t_{\text{erg}}$ . Indeed, in the perturbative regime, where  $t_{\text{erg}} \ll t_{\text{prt}}$ , it will be argued that effectively  $\tau_c \gg t_{\text{erg}}$ . In the perturbative regime we are not able to give a general mathematical proof for having an effective  $\tau_c$  such that the separation of time scales requirement ( $\tau_c \ll t_{\text{prt}}$ ) is being satisfied. However, we are going to demonstrate that a crossover to a diffusive-growth of the second moment happens *before* the breaktime  $t_{\text{prt}}$ . The *assumption* that the diffusive behavior *persists* beyond  $t_{\text{prt}}$  with the *same* diffusion coefficient is the cornerstone of the common FGR picture. We are not going to study in this paper the general conditions for having stochastic-like behavior.

The derivation of the classical  $\mathcal{FD}$  relation consists of two steps: The *first step* establishes the local diffusive behavior for short ( $t \ll t_{\text{frc}}$ ) time scales, and  $D_E$  is determined; The *second step* establishes the global stochastic behavior on large ( $t \gg t_{\text{erg}}$ ) time scales. The various time scales involved are illustrated in Fig.4. The



**Figure 4.** Illustration of the various time scales involved in constructing either classical, semiclassical or perturbation theory of dissipation. We use the notation  $\tau_{\text{SC}} = \delta x_{\text{SC}}/V$ . The accompanying table summarizes the associated requirements for the applicability of each of those theories. Note that the quantum mechanical definitions of slowness and of fastness are not complementary. Note also that slowness in the classical sense is always assumed. The rest of this paper (Sections 9-20) is devoted to the study of the ballistic-diffusive crossover. This crossover is ‘captured’ either by perturbation theory or by the semiclassical theory, provided the respective slowness or fastness conditions are satisfied. For simplicity we assume a generic system where  $\tau_{\text{cl}}$  can be identified with  $t_{\text{erg}}$ . The persistence of the stochastic behavior for arbitrarily long times is assumed. We are not going to study in this paper the general conditions for having such long-time stochastic behavior.

validity of the classical derivation depends on the slowness condition (10). The validity of the analogous QM theory is further restricted by the quantal slowness condition (23). However, an optional derivation of the  $\mathcal{FD}$  relation in the QM case can be based on semiclassical considerations. The limitations of the latter strategy are illustrated in Fig.4, and further discussed in the next section.

## 9. The semiclassical picture and detailed QCC

The main objects of our discussion are the transition probability kernel  $P_t(n|m)$  and the parametric kernel  $P(n|m)$  which have been introduced in the previous section. Recall that we are measuring phase-space volume ( $n=\Omega(E)$ ) in units of  $(2\pi\hbar)^d$ . This way we can obtain a ‘classical approximation’ for the QM kernel, simply by making  $n$  and  $m$  integer variables. If the ‘classical approximation’ is similar to the QM kernel, then we say that there is *detailed* QCC. If only the second-moment is similar, then we

say that there is *restricted* QCC. In the present section we are going to discuss the conditions for having detailed QCC, using simple *semiclassical* considerations. In the next paragraph we discuss the conditions for having detailed QCC in the computation of the parametric kernel  $P(n|m)$ . Then we discuss the further restrictions on detailed QCC, that are associated with the computation of the actual kernel  $P_t(n|m)$ .

Wigner function  $\rho_{n,x}(Q, P)$ , unlike its classical microcanonical analog, has a non-trivial transverse structure. For a curved energy surface the transverse profile looks like Airy function and it is characterized by a width [23]

$$\Delta_{\text{SC}} = \left( \varepsilon_{\text{cl}} \left( \frac{\hbar}{\tau_{\text{cl}}} \right)^2 \right)^{1/3} \quad (47)$$

where  $\varepsilon_{\text{cl}}$  is a classical energy scale. For the ‘piston’ example  $\varepsilon_{\text{cl}} = E$  is the kinetic energy of the gas particle. The classical  $P(n|m)$  has a dispersion

$$\delta E_{\text{cl}} = \sqrt{\left\langle \left( \frac{\partial \mathcal{H}}{\partial x} \right)^2 \right\rangle_{\text{E}}} \delta x \quad (48)$$

which characterizes the transverse distance between the intersecting energy-surfaces  $|m(x)\rangle$  and  $|n(x+\delta x)\rangle$ . In the generic case, it should be legitimate to neglect the transverse profile of Wigner function provided  $\delta E_{\text{cl}} \gg \Delta_{\text{SC}}$ . This condition can be cast into the form  $\delta x \gg \delta x_{\text{SC}}$  where

$$\delta x_{\text{SC}} = \frac{\Delta_{\text{SC}}}{\sqrt{\nu_{\text{E}}/\tau_{\text{cl}}}} \propto \hbar^{2/3} \quad (49)$$

For the ‘piston’ example see [14]. Another important parametric scale is defined in a similar fashion: We shall see that it is *not* legitimate to ignore the transverse profile of Wigner function if  $\delta E_{\text{cl}} < \Delta_b$ . This latter condition can be cast into the form  $\delta x \ll \delta x_{\text{prt}}$  where

$$\delta x_{\text{prt}} = \frac{\Delta_b}{\sqrt{\nu_{\text{E}}/\tau_{\text{cl}}}} = \frac{2\pi\hbar}{\sqrt{\nu_{\text{E}}\tau_{\text{cl}}}} \quad (50)$$

Typically the two parametric scales are well separated ( $\delta x_{\text{prt}} \ll \delta x_{\text{SC}}$ ). If we have  $\delta x \ll \delta x_{\text{prt}}$  then the parametric kernel  $P(n|m)$  is characterized by a perturbative core-tail structure which is illustrated in Fig.3 and further discussed in the next section. If we have  $\delta x \gg \delta x_{\text{SC}}$  then the transverse profile of Wigner function can be ignored, and we get detailed QCC. Obviously, ‘detailed QCC’ does not mean complete similarity. The classical kernel is typically characterized by various non-Gaussian features, such as sharp cutoffs, delta-singularities and cusps. These features are expected to be smeared in the QM case. The discussion of the latter issue is beyond the scope of the present paper [14].

We turn now to discuss the actual transition probability kernel  $P_t(n|m)$ . Here we encounter a new restriction on QCC: The evolving surface  $\mathcal{U}(t)|m\rangle$  becomes more and more convoluted as a function of time. This is because of the mixing behavior that characterizes chaotic dynamics. For  $t \gg t_{\text{scl}}$  the intersections with a given instantaneous energy surface  $|n\rangle$  become very dense, and associated QM features can no longer be ignored. The time scale  $t_{\text{scl}}$  can be related to the failure of the stationary phase approximation [17].

The breaktime scale  $t_{\text{scl}}$  of the semiclassical theory is analogous to the breaktime scale  $t_{\text{prt}}$  of perturbation theory, as well as to the breaktime scale  $t_{\text{irc}}$  of the classical theory. In order to establish the crossover from ballistic to diffusive energy spreading using a semiclassical theory we should satisfy the condition  $\tau_{\text{cl}} < t_{\text{scl}}$ . This velocity-independent condition is not very restrictive. On the other hand we should also

satisfy the condition  $\delta x \gg \delta x_{\text{SC}}$ , with  $\delta x = V\tau_{\text{cl}}$ . The latter condition implies that the applicability of the semiclassical theory is restricted to relatively high velocities. We can define:

$$v_{\text{SC}} = \sqrt{D_{\text{E}} \tau_{\text{cl}}} / \Delta_{\text{SC}} \quad (51)$$

If  $v_{\text{SC}} \gg 1$  then the above semiclassical analysis is applicable in order to analyze the crossover from ballistic to diffusive energy spreading.

## 10. The perturbative picture and restricted QCC

Detailed QCC between the quantal  $P(n|m)$  and the classical  $P(n|m)$  is not guaranteed if  $\delta x < \delta x_{\text{SC}}$ . A-fortiori, this statement holds also for  $P_t(n|m)$ . For sufficiently small parametric changes  $\delta x$ , or for sufficiently short times  $t$ , perturbation theory becomes a useful tool for the analysis of these kernels. A detailed formulation of perturbation theory is postponed to later sections. In the present section we are going to sketch the main observations. We are going to argue that for small enough  $\delta x$  there is no *detailed* QCC between the quantal and the classical kernels, but there is still *restricted* QCC that pertains to the second moment of the distributions. Large enough  $\delta x$  is a necessary condition for getting detailed QCC. The following paragraph discuss the parametric evolution of  $P(n|m)$ , and the rest of this section discuss the actual evolution of  $P_t(n|m)$ .

For extremely small  $\delta x$  the parametric kernel  $P(n|m)$  has a standard ‘first-order’ perturbative structure, namely:

$$P(n|m) \approx \delta_{nm} + \text{Tail}(n-m) \quad \text{for } \delta x \ll \delta x_c^{\text{qm}} \quad (52)$$

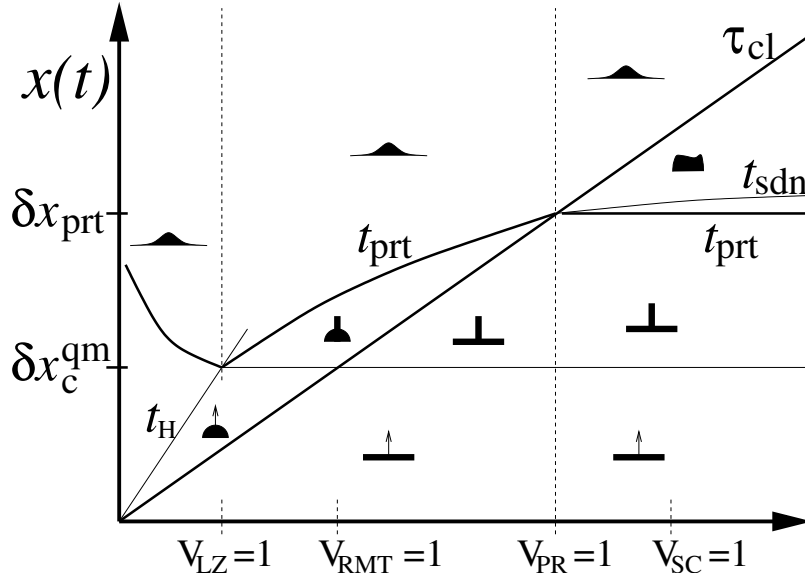
where  $\delta x_c^{\text{qm}}$  is defined as parametric change that is needed in order to mix neighboring levels. For larger values of  $\delta x$  neighbor levels are mixed non-perturbatively and consequently we have a more complicated spreading profile:

$$P(n|m) \approx \text{Core}(n-m) + \text{Tail}(n-m) \quad \text{for } \delta x \ll \delta x_{\text{prt}} \quad (53)$$

In the perturbative case ( $\delta x \ll \delta x_{\text{prt}}$ ) the second moment of  $P(n|m)$  is generically determined by the ‘tail’. It turns out that the QM expression for the second-moment is classical look-alike, and consequently *restricted* QCC is satisfied. The *core* of the quantal  $P(n|m)$  is of non-perturbative nature. The *core* is the component that is expected to become similar (eventually) to the classical  $P(n|m)$ . A large perturbation  $\delta x \gg \delta x_{\text{prt}}$  makes the *core* spill over the perturbative *tail*. If we have also  $\delta x \gg \delta x_{\text{SC}}$ , then we can rely on detailed QCC in order to estimate  $P(n|m)$ . The parametric scales  $\delta x_c^{\text{qm}}$  and  $\delta x_{\text{prt}}$  are easily estimated in case of the ‘piston’ example. The displacement which is needed in order to mix levels is much smaller than De-Broglie wavelength, namely  $\delta x_c^{\text{qm}} \approx (\lambda_{\text{E}}^{d+1}/\text{Area})^{1/2}$ . The displacement which is needed in order to mix core and tail is much larger than De-Broglie wavelength, namely  $\delta x_{\text{prt}} \approx (\tau_{\text{col}}/\tau_{\text{cl}})^{1/2}\lambda_{\text{E}}$ . For a more careful discussion of these parametric scales see [14, 15] and the concluding section.

The dynamical evolution of  $P_t(n|m)$  is related to the associated parametric evolution of  $P(n|m)$ . We can define a perturbative time scale  $t_{\text{prt}}$  which is analogous to  $\delta x_{\text{prt}}$ . For  $t \ll t_{\text{prt}}$  the kernel  $P_t(n|m)$  is characterized by a core-tail structure that can be analyzed using perturbation theory. In particular we can determine the second moment of the energy distribution, and we can establish *restricted* QCC. If the second moment for the core-tail structure is proportional to  $t^2$ , we shall say that there is a ballistic-like behavior. If it is proportional to  $t$ , we shall say that there is a diffusive-like behavior. *In both cases the actual energy distribution is not classical-like*, and therefore the term ‘ballistic’ and ‘diffusive’ should be used with care. We are going now to give a brief overview of the various scenarios in the time evolution of





**Figure 5.** The various crossovers in the time evolution of  $P_t(n|m)$ . The vertical axis is  $x(t) = Vt$ . The parametric scales  $\delta x_c^{\text{qm}}$  and  $\delta x_{\text{prt}}$  are indicated by horizontal lines. The horizontal axis is the velocity  $V$ . It is divided by vertical dashed lines to various velocity regimes. In each velocity regime there is a different dynamical route. The various crossovers are explained in the text and the various symbols are easily associated with having either Gaussian or some non-Gaussian spreading profile. In particular the perturbative spreading profile is either with or without non-trivial core, and its tail is either band-limited or resonance-limited.

$P_t(n|m)$ . These are illustrated in Fig.5. In later sections we give a detailed account of the theory.

For *slow velocities* such that  $\tau_{\text{cl}} \ll t_{\text{prt}}$ , there is a crossover from ballistic-like spreading to diffusive-like spreading at  $t \sim \tau_{\text{cl}}$ . In spite of the lack of detailed QCC there is still restricted QCC as far as this ballistic-diffusive crossover is concerned. If the breakdown of perturbation theory happens before the Heisenberg time ( $t_{\text{prt}} \ll t_{\text{H}}$ ) it is implied that there is a second crossover at  $t \sim t_{\text{prt}}$  from a diffusive-like spreading to a genuine diffusive behavior. Once a stochastic behavior is established, the time scale  $t_{\text{H}}$  for recurrences becomes non-effective, and we expect a long-time classical-like behavior.

*extremely slow velocities* are defined by the inequality  $t_{\text{H}} \ll t_{\text{prt}}$ . This inequality implies that there are QM recurrences *before* the expected crossover from diffusive-like spreading to genuine-diffusion. This is the QM adiabatic regime. In the  $t \rightarrow \infty$  limit Landau-Zener transitions will dominate the energy spreading, and consequently neither detailed nor restricted QCC is a-priori expected [9].

For *fast velocities* we have  $t_{\text{prt}} \ll \tau_{\text{cl}}$ . There is a crossover at  $t \sim t_{\text{prt}}$  from ballistic-like spreading to a genuine ballistic behavior, and at  $t \sim \tau_{\text{cl}}$  there is a second crossover from genuine-ballistic to genuine-diffusive spreading. The description of this classical-type crossover is out-of-reach for perturbation theory, but we can use the semiclassical picture instead. Note that the semiclassical definition of ‘fastness’ and the perturbative definition of ‘slowness’ imply that there is a ‘gap’ between the corresponding regimes. However, the interpolation is smooth, and therefore for simple systems surprises are not expected.

## 11. Actual versus Parametric Evolution

The QM time evolution is governed by the time dependent Schroedinger equation with the time dependent Hamiltonian  $\mathcal{H}(x(t))$ . In practice it is quite unnatural to use a fixed basis. For example, in case of the ‘piston’ example one may propose to use the fixed-basis that consists of the eigenfunctions of the empty cavity. However, the matrix elements of the ‘piston’ may be very large and even infinite if we assume impenetrable walls. Thus, it is much more natural to use the so called adiabatic basis, though the time evolution is not necessarily of adiabatic nature. The evolving state-vector is expanded as follows:

$$|\psi(t)\rangle = \sum_n a_n(t) |n(x(t))\rangle \quad (54)$$

Using standard manipulation we obtain the Schroedinger-like equation

$$\frac{da_n}{dt} = -\frac{i}{\hbar} E_n a_n - \frac{i}{\hbar} \sum_m \mathbf{W}_{nm}(x(t)) a_m \quad (55)$$

Were the off diagonal elements of  $\mathbf{W}_{nm}$  are

$$\mathbf{W}_{nm} = \frac{\hbar}{i} \left\langle n \left| \frac{d}{dt} \right| m \right\rangle = i \frac{\hbar \dot{x}}{E_n - E_m} \left\langle n \left| \frac{\partial \mathcal{H}}{\partial x} \right| m \right\rangle \quad (56)$$

and we use the ‘gauge’ convention  $\mathbf{W}_{nm}=0$  for  $n=m$ . (Only one parameter is being changed and therefore Berry’s phase is not an issue).

Equation (55) will be now our starting point. It is defined in terms of  $\mathbf{W}_{nm}(x)$  and in terms of a set of numbers  $\{E_n\}$ . Note that as long as  $t \ll t_H$  we can *ignore* the dependence of  $E_n$  on the changing parameter  $x$ . The formal solution of (55) will be written as follows:

$$a_n(t) = \sum_m \mathbf{U}_{nm}(t) a_m(0) \quad (57)$$

If all the  $E_n$  are set equal to the same constant, (or without loss of generality to zero), then (55) describes the time evolution of a frozen wavefunction. In other words, (55) without the  $\{E_n\}$  is equivalent to the trivial equation  $d\psi/dt = 0$ . In this special case the formal solution (57) will be written with  $\mathbf{T}_{nm}(x(t))$  instead of  $\mathbf{U}_{nm}(t)$ . Note that if the  $\{E_n\}$  are taken away from (55), then  $\dot{x}$  can be scaled out and therefore the  $x$  dependence rather than the  $t$  dependence become significant. The transition probability kernel and the parametric kernel can be written as:

$$P_t(n|m) = |\mathbf{U}_{nm}(t)|^2 = |\langle n(x(t)) | \mathbf{U}(t) | m(x(0)) \rangle|^2 \quad (58)$$

$$P(n|m) = |\mathbf{T}_{nm}(x)|^2 = |\langle n(x) | m(x(0)) \rangle|^2 \quad (59)$$

From now on we shall refer to the  $t$ -dependent evolution which is represented by  $\mathbf{U}_{nm}(t)$  as the *actual evolution* (AE). To the  $t$ -dependent evolution which is represented by  $\mathbf{T}_{nm}(x(t))$  will shall refer as *parametric evolution* (PE). For PE the velocity  $\dot{x} = V$  plays no role, and it can be scaled out from the above equation. Consequently, for PE, parametric scales and temporal scales are trivially related via the scaling transformation  $\delta x = V\tau$ .

It is important to realize that in a certain sense, defined below, the AE coincided with the PE for short times  $t \ll t_{\text{sdn}}$ . This is the QM-*sudden* approximation. The detailed picture is as follows: We start with some initial state  $|m\rangle$ . After time  $t$  there will be some non-vanishing probability to find the system in a certain energy range  $\delta E(t)$  around  $E_m$ . As long as  $\delta E(t) \ll \hbar/t$  the corresponding energy levels  $E_n$  within  $\delta E$  are not resolved. The latter condition defines a time interval  $t \ll t_{\text{sdn}}$ . By definition, for  $t \ll t_{\text{sdn}}$  it is as if the energy-levels were degenerated. Therefore we can say that the AE coincides with the PE, implying that the evolving state (54) remains approximately unchanged. The QM sudden approximation will be further discussed in Sec.19.

## 12. Application of perturbation theory

We can use Equation (55) as a starting point for a standard first-order perturbation theory (FOPT). For short times, such that  $P_t(m|m) \sim 1$ , the transition probability from level  $m$  to level  $n$  is determined by the coupling strength  $|\mathbf{W}_{nm}|^2$ , by the energy difference  $(E_n - E_m)$  and by the correlation function  $F(\tau)$ . The latter describes loss of correlation between  $\mathbf{W}_{nm}(x(0))$  and  $\mathbf{W}_{nm}(x(t))$ . It is defined via

$$\langle \mathbf{W}_{nm}^*(t+\tau) \mathbf{W}_{nm}(t) \rangle = |W_{nm}|^2 F(\tau) \quad (60)$$

with the convention  $F(0) = 1$ . Using FOPT one obtains the following result:

$$\begin{aligned} P_t(n|m) &= \left| \int_0^t \frac{\mathbf{W}_{nm}(t')}{\hbar} e^{i\frac{E_n - E_m}{\hbar} t'} dt' \right|^2 \\ &= \left( \frac{W_{nm}}{\hbar} \right)^2 \int_0^t \int_0^t dt_2 dt_1 F(t_2 - t_1) e^{i\frac{E_n - E_m}{\hbar} (t_2 - t_1)} \\ &= t \tilde{F}_t \left( \frac{E_n - E_m}{\hbar} \right) \times \left( \frac{W_{nm}}{\hbar} \right)^2 \quad \text{for } n \neq m \end{aligned} \quad (61)$$

The function  $\tilde{F}_t(\omega)$  describes the spectral content of the perturbation. For a *constant* perturbation ( $F(\tau) = 1$ ) it is just given by equation (25). For a *noisy* perturbation  $F(\tau)$  is characterized by some finite correlation-time  $\tau_c$ , and therefore the definition of  $\tilde{F}_t(\omega)$  is modified as follows:

$$\tilde{F}_t(\omega) = \begin{cases} t \cdot (\text{sinc}(\omega t/2))^2 & \text{for } t < \tau_c \\ \tilde{F}(\omega) & \text{for } t > \tau_c \end{cases} \quad (62)$$

where  $\tilde{F}(\omega)$  is the Fourier transform of the correlation function  $F(\tau)$ . Now it is a simple matter to calculate the *second-moment* of the spreading:

$$\delta E^2 = \sum_n (E_n - E_m)^2 P_t(n|m) = V^2 t \int_{-\infty}^{+\infty} \frac{d\omega}{2\pi} \tilde{C}_E(\omega) \tilde{F}_t(\omega) \quad (63)$$

This result coincides with the linear-response result (24) only if the coupling matrix-elements could have been treated as *constant* in time, meaning  $F(\tau)=1$  and accordingly  $\tau_c = \infty$ . For  $t > \tau_c$  it becomes *formally equivalent* to the FGR result (31). However, a *practical equivalence* seems unlikely because  $F(\tau)$  of (60) is not necessarily determined by the correlations of the external driving source. The critical discussion of this point is going to be the main issue of the subsequent sections.

In order to use (63) we should determine how  $F(\tau)$  look like, and in particular we should determine what is the correlation-time  $\tau_c$ . We postpone this discussion, and assume that  $F(\tau)$  and hence  $\tau_c$  are known from some calculation. The total transition probability is  $p(t) = \sum'_n P(n|m)$ , where the prime indicates omission of the term  $n = m$ . FOPT is valid as long as  $p(t) \ll 1$ . This defines a brektime  $t'_{\text{prt}}$  for the *standard* FOPT treatment. The above derivation imply that we can trust (63) only during the short time  $t \ll t'_{\text{prt}}$ . However, later we shall argue that with a proper (modified) definition of  $F(\tau)$  we can trust (63) during a longer time  $t \ll t_{\text{prt}}$ . The brektime  $t_{\text{prt}}$  will be determined by using an *improved* perturbation theory (IMPT).

It is now possible to formulate the conditions for having *restricted* QCC. By 'restricted' QCC we mean that only the *second-moment* of the spreading (63) is being considered. It is essential to distinguish between two different possible scenarios:

$$\text{Resonance-limited transitions:} \quad \tau_c \gg \tau_{\text{cl}} \quad (64)$$

$$\text{Band-limited transitions:} \quad \tau_c \ll \tau_{\text{cl}} \quad (65)$$

For resonance-limited transitions, finite  $\tau_c$  has no consequence as far as  $\delta E^2$  is concerned. The crossover to diffusive behavior  $\delta E^2 \propto t$  will happen at  $t \sim \tau_{\text{cl}}$ . This

diffusive behavior will persist for  $t > \tau_c$  with the same diffusion coefficient. On the other hand, for band-limited transitions we will have at  $t \sim \tau_c$  a pre-mature crossover from ballistic to diffusive behavior. Consequently the classical result will be suppressed by a factor  $(\tau_c/\tau_{cl}) \ll 1$ . This is due to the fact that the transitions between levels are limited not by the resonance width (embodied by  $\tilde{F}(\omega)$ ), but rather by the band-width of the coupling matrix elements (embodied by  $\tilde{C}_E(\omega)$ ).

We have realized that the perturbative result (63) can be used in order to establish a *diffusive* growth of the *second moment*. Obviously the applicability of this picture requires a separation of time scales:

$$\mathbf{FGR-condition:} \quad \text{Either } \tau_{cl} \text{ or } \tau_c \ll t_{prt} \quad (66)$$

The long time *stochastic* behavior of the spreading is determined by the short-time dynamics, as explained in Section 8. The FGR condition guarantees that the *diffusive* growth of the *second-moment* is established *before* the breakdown of the short-time analysis. Therefore, the correct determination of the breaktime  $t_{prt}$  is extremely important, and it is going to be the main issue of the subsequent sections.

### 13. The applicability regime of the standard FOPT treatment

In order to have practical estimates for applicability regime of the standard FOPT treatment, we should look on the matrix  $\mathbf{W}_{nm}$ . This matrix is banded, and its elements satisfy:

$$\left\langle \left| \frac{\mathbf{W}_{nm}}{\hbar} \right|^2 \right\rangle \approx \left( \frac{V}{\delta x_c^{qm}} \right)^2 \frac{1}{(n-m)^2} \quad \text{for } |n-m| < b/2 \quad (67)$$

where  $\delta x_c^{qm} = \Delta/\sigma$ . From the above expression, once used in (61) for the calculation of the kernel  $P(n|m)$ , it follows that  $\delta x_c^{qm}$  is the parametric change which is required in order to mix neighboring levels. Similarly, in the calculation of  $P_t(n|m)$  the related  $\tau_c^{qm} = \delta x_c/V$  is the time which is required in order to mix neighboring levels. Given two distant levels  $n$  and  $m$ , and taking the mixing on ‘‘small’’ scale into account, one realizes that  $\delta x_c^{qm}$  also determines the correlation time  $\tau_c = \tau_c^{qm}$  of the matrix-element  $\mathbf{W}_{nm}(x(t))$ , as defined in (60). These observations can be summarized as follows:

$$t'_{prt} = \tau_c = \tau_c^{qm} \quad \text{for the standard FOPT.} \quad (68)$$

The standard perturbative structure (52) of either  $P(n|m)$  or  $P_t(n|m)$  is maintained as long as neighboring levels are not being mixed. This structure obviously does not correspond to the classical structure since it is characterized by the non-classical energy scale  $\Delta_b$ . Still, there is *restricted* QCC which is implied by (63).

A sufficient condition for the applicability of the *standard* FOPT treatment is  $v_{RMT} \ll 1$ . The argument goes as follows: By definition  $v_{RMT} \ll 1$  implies  $\tau_{cl} \ll \tau_c^{qm}$ . Using (68) we observe that it is equivalent to  $\tau_{cl} \ll t'_{prt}$ . By definition  $t_{prt}$  is either equal or larger than  $t'_{prt}$ . Therefore the FGR condition (66) is satisfied. The converse however is not true. Having  $v_{RMT} \gg 1$  does not imply that the FGR condition cannot be satisfied. Therefore, for  $v_{RMT} \gg 1$ , we cannot tell on the basis of the *standard* FOPT treatment whether or when there is a crossover to a diffusive behavior. We shall try to overcome this difficulty in the next sections.

### 14. The over-simplified RMT (ORMT) picture

Recall that the matrix  $\mathbf{W}_{nm}$  is a banded. The bandwidth  $b=1, 3, \dots$  corresponds to diagonal, tridiagonal matrix and so on. In the spirit of RMT we can think of  $\mathbf{W}_{nm}$  as a particular realization which is taken out from some large ensemble of (banded)

random matrices. In order to go beyond standard FOPT it is essential to further specify the *cross-correlation between matrix elements*. Following [10] the simplest statistical assumption is *absence* of cross-correlations, namely,

$$\langle \mathbf{W}_{n'm'}^*(t+\tau) \mathbf{W}_{nm}(t) \rangle = 0 \quad \text{if } \{n', m'\} \neq \{n, m\} \quad (69)$$

Equation (55) with the statistical assumptions (69) and (60), where  $\tau_c = \tau_c^{\text{qm}}$ , is a well defined RMT model. We shall refer to it as the over-simplified RMT (ORMT) picture. The main observation of [10] can be summarized as follows: The FOPT result (63), assuming an ORMT picture, can be trusted for classically long times. Namely,

$$t'_{\text{prt}} = t_{\text{fc}} \quad \text{and} \quad \tau_c = \tau_c^{\text{qm}} \quad \text{for the ORMT picture.} \quad (70)$$

The ORMT picture reduces to FOPT and implies restricted QCC provided  $v_{\text{RMT}} \ll 1$ . However, this condition is *not* satisfied in the classical limit ( $\hbar \rightarrow 0$ ). In the classical limit  $v_{\text{RMT}} \gg 1$ , and consequently transitions are band-limited. In particular it follows from (63), that the classical diffusion ( $D_{\text{E}}^{\text{cl}}$ ) is suppressed by a factor  $\tau_c/\tau_{\text{cl}}$ , leading to

$$D_{\text{E}}^{\text{ORMT}} \approx \frac{1}{v_{\text{RMT}}} D_{\text{E}}^{\text{cl}} \quad \text{for } v_{\text{RMT}} \gg 1 \quad (71)$$

This result, which is the main result of [10], is obviously inconceivable, because it is implied that the classical limit does not coincide with the classical result, and that the correspondence principle is actually violated.

The ORMT picture predicts (for  $v_{\text{RMT}} \gg 1$ ) a premature crossover from ballistic to diffusive behavior once  $\delta x$  becomes larger than  $\delta x_c^{\text{qm}}$ . It is important to realize that (71), if it were true, would reflect a property of PE. This statement becomes more transparent if we write:

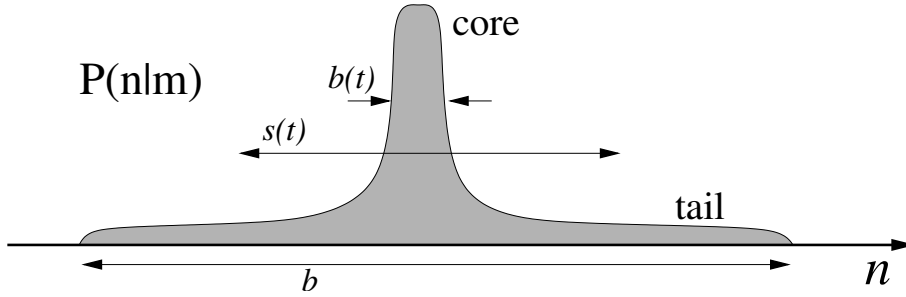
$$\delta E^2 \Big|_{\text{ORMT}} = 2D_{\text{E}}^{\text{ORMT}} \times t \approx \left\langle \left( \frac{\partial \mathcal{H}}{\partial x} \right)^2 \right\rangle_{\text{E}} \delta x_c^{\text{qm}} \times \delta x \quad (72)$$

Exactly the same result would be obtained if we start with (55) without the the first term in the right hand side. The value of  $V$  has no significance in the above analysis.

## 15. The core-tail structure

There is no detailed QCC between the classical and the quantal  $P_t(n|m)$  for short times. We are going to explain that for a limited time  $P_t(n|m)$  consists of a *core* whose width will be denoted by  $b(t)$ , and a *tail* whose main component is contained within the bandwidth  $b$ . In order to analyze this core-tail structure we are going to use an improved perturbation theory (IMPT). The IMPT treatment assumes that out-of-band transitions ( $b/2 < |n-m|$ ) can be neglected. The IMPT is useful as long as the *second-moment* of the energy distribution is predominated by the tail component. This determines the breaktime  $t_{\text{prt}}$ . The breakdown of IMPT at  $t \sim t_{\text{prt}}$  happens once the core spills over the tail region, and the FOPT-like structure of  $P_t(n|m)$  is completely washed away.

It is important to have a proper intuitive understanding of how the *core* is being formed. For  $t \ll \tau_c^{\text{qm}}$  we have  $P_t(m|m) \sim 1$  and  $P_t(n|m) \ll 1$  for  $n \neq m$ . It means that the core width is  $b(t) = 1$ . For  $t \sim \tau_c^{\text{qm}}$  few levels are expected to be mixed by the perturbation, meaning that  $b(t) > 1$ . We may have the tendency to associate this mixing with an avoided crossing. However, this aspect should not be over-emphasized. The mixing of neighboring levels is *not* conditioned by having exceptionally small energy difference (having  $(E_{m+1} - E_m) \ll \Delta$  is not required). Moreover, one should not over-emphasize the importance of near-neighbor transitions, unless  $v_{\text{LZ}} \ll 1$ . (See further discussion of the QM-adiabatic regime in Sec.20). If near-neighbor transitions were the dominant mechanism for energy spreading, it would



**Figure 6.** Schematic illustration of a generic core-tail spreading profile. The core-width  $b(t)$  is defined by the participation-ratio. The second-moment should satisfy  $b(t) \ll s(t) \ll b$ , where  $b$  is that bandwidth. In case of  $P_t(n|m)$  the tail becomes (for  $t > \tau_{c1}$ ) resonance-limited rather than band-limited. In the resonance-limited case the bandwidth  $b$  in the above figure should be replaced by  $(\hbar/t)/\Delta$ , and accordingly the requirement is  $b(t) \ll s(t) \ll (\hbar/t)/\Delta$ .

imply that  $b(t) \approx (t/\tau_c^{\text{qm}})$ . Rather, we shall argue that the core develops much more rapidly, namely  $b(t) \approx (t/\tau_c^{\text{qm}})^2$ .

It is also important to have a proper intuitive understanding of how the *tail* is being formed. Let us assume for simplicity that only three levels  $m = 1$ ,  $m = 2$  and  $n = 100$  are actually coupled by matrix elements. Let us start at  $t = 0$  with all the probability concentrated in  $m = 1$ . As we go at  $t = t_1$  via an avoided-crossing of  $m = 1$  and  $m = 2$ , the matrix element  $\mathbf{W}_{n,1}$  may change sign. This change of sign may be viewed as a loss of correlations. However, at the same time, assuming a diabatic transition, almost all the probability is transferred to  $m = 2$  in such a way that  $\mathbf{W}_{n,2}a_2$  at  $t > t_1$  is strongly correlated with  $\mathbf{W}_{n,1}a_1$  at  $t < t_1$ . It is implied that the effective correlation time  $\tau_c$  for  $m \rightarrow n$  transitions is larger than the time between avoided crossings. This is not captured by the statistical assumption (69) of the previous section. A proper transformation, that effectively removes the in-core transitions between  $m$ -states, can be used for the purpose of tail-formation analysis. The associated perturbative treatment is characterized by an effective  $\tau_c \gg \tau_c^{\text{qm}}$  as well as by  $t'_{\text{prt}} \gg \tau_c^{\text{qm}}$ .

For  $t > \tau_c^{\text{qm}}$  neighboring levels are being mixed and consequently the transition kernel acquires a non-trivial core-tail structure which is illustrated in Fig.6. The expression for  $P_t(n|m)$  can be written schematically as follows:

$$P_t(n|m) \approx \text{Core}(n-m) + \text{Tail}(n-m) \quad \text{for } t \ll t_{\text{prt}} \quad (73)$$

The kernel is characterized now by two scales:

$$b(t) = \text{core width} = \left( \sum_n (P_t(n|m))^2 \right)^{-1} \quad (74)$$

$$s(t) = \text{spreading} = \left( \sum_n (n-m)^2 P_t(n|m) \right)^{-1/2} \quad (75)$$

such that  $b(t) \ll s(t) \ll b$ . For  $t < \tau_c^{\text{qm}}$  we have a trivial core with  $b(t) \approx 1$ , whereas for  $t \gg \tau_c^{\text{qm}}$  we have a non-trivial core with  $b(t) \gg 1$ . The matrix elements satisfy  $\langle |\mathbf{W}_{nm}|^2 \rangle \propto 1/(n-m)^2$ . We shall see that in the ‘band-limited tail’ case we have  $P_t(n|m) \sim \text{const}/(n-m)^2$  up to the cutoff  $b$ , while for the ‘resonance-limited tail’ case we have  $P_t(n|m) \sim \text{const}/(n-m)^2$  up to the cutoff  $(\hbar/t)/\Delta$ . One should realize that the power-law behavior of the tail is ‘fast’ enough in order to guarantee that  $b(t)$  is independent of the tail’s cutoff. The cutoff does not have any effect on the evolving

core. On the other hand, the second moment  $s(t)$ , unlike  $b(t)$ , is predominantly determined by the tail's cutoff, and it is independent of the core structure.

## 16. An improved perturbation theory (IMPT)

In order to extend perturbation theory beyond  $\tau_c^{\text{qm}}$  it is essential to eliminate the non-perturbative transitions within the core. This can be done by making a transformation to an appropriate basis as follows:

$$a_n(t) = \sum_m \tilde{\mathbf{T}}_{nm} c_m(t) \quad (76)$$

$$\tilde{\mathbf{T}}_{nm} = \mathbf{T}_{nm} \quad \text{if } |n-m| < b'/2, \text{ else zero.} \quad (77)$$

The amplitudes  $c_n(t)$  satisfy the same Schroedinger equation as the  $a_n(t)$ , with a transformed matrix  $\tilde{\mathbf{W}}$ . The general expression for  $\tilde{\mathbf{W}}$  is

$$\tilde{\mathbf{W}} = \tilde{\mathbf{T}}^\dagger \mathbf{W} \tilde{\mathbf{T}} - i\hbar \tilde{\mathbf{T}}^\dagger (d\tilde{\mathbf{T}}/dt) + \tilde{\mathbf{T}}^\dagger \mathbf{E} \tilde{\mathbf{T}} \quad (78)$$

where  $\mathbf{E}$  is a diagonal matrix of the energies. This is a quite complicated expression. However, we are interested only in the core-to-tail transitions for which

$$(\tilde{\mathbf{W}})_{nm} = (\tilde{\mathbf{T}}^\dagger \mathbf{W} \tilde{\mathbf{T}})_{nm} \quad \text{for } |n-m| > b' \quad (79)$$

(no approximation is involved). Once this transformation is performed the 'new' Schroedinger equation will be characterized by a new correlation time  $\tau_c$  and by a new perturbative time  $t'_{\text{prt}}$ . Both  $\tau_c$  and  $t'_{\text{prt}}$  will depend on the free parameter  $b'$ . Our choice of the course-graining parameter  $b'$  is not completely arbitrary. The restrictions are:

- Unitarity is approximately preserved:  $b(t) \ll b'$ .
- Core-to-Tail transitions are preserved:  $b' \ll b$ .
- Long effective correlation time is attained:  $\tau_{\text{cl}} \ll \tau_c$

The feasibility of the last requirement deserves further discussion. Only matrix elements with  $|n-m| \gg b'$  are of interest, and therefore in the multiplication  $(\tilde{\mathbf{T}}^\dagger)_{n'n} (\mathbf{W})_{nm} (\tilde{\mathbf{T}})_{mm'}$  we can substitute (56) with  $(E_n - E_m)$  replaced by  $(E_{n'} - E_{m'})$ . As  $b'$  becomes closer to  $b$ , the matrix elements  $(\tilde{\mathbf{W}})_{n'm'}$  become correlated on a time scale of the order  $\tau_c^{\text{cl}}$ . This is because  $b' = b$  implies transformation to an  $x$ -independent basis. The time scale  $\tau_c^{\text{cl}}$  has been defined in Sec.3. As we change  $b'$  from  $b$  back to smaller values, we expect  $\tau_c$  to become smaller. By continuity, we expect no difficulty in satisfying the conditions  $b' \ll b$  and  $\tau_c \gg \tau_{\text{cl}}$  simultaneously. The validity of the improved perturbative treatment is further discussed in the next section.

The usefulness of the above transformation stems from the fact that due to the elimination of non-perturbative transitions within the core,  $t'_{\text{prt}}$  becomes much longer than  $\tau_c^{\text{qm}}$ . At the same time the information which is required in order to determine the second moment  $s(t)$  is not lost. We have  $|\tilde{\mathbf{W}}_{nm}| \approx |\mathbf{W}_{nm}|$  for core-to-tail transitions, and a practical approximation for the 'renormalized' spreading profile is

$$P_t(n|m) \sim \delta_{nm} + t \tilde{E}_t \left( \frac{E_n - E_m}{\hbar} \right) \times \left( \frac{1}{\tau_c^{\text{qm}}} \right)^2 \frac{1}{(b')^2 + (n-m)^2} \quad (80)$$

Breakdown of the improved perturbative treatment happens once the total transition probability becomes non-negligible (of order 1). Thus

$$t'_{\text{prt}} = (b')^{1/2} \times \tau_c^{\text{qm}} \quad (81)$$

The behavior for  $|n-m| \leq b'$  is an artifact of the transformation and contains false information. However, for the calculation of the second moment only the tail is

significant. The tail is not affected by our transformation and therefore we will obtain the *same* result (63) for  $\delta E^2$  with one important modification: a different effective value for  $\tau_c$ . Moreover, since  $b'$  is chosen such that  $\tau_c \gg \tau_{cl}$ , it follows that the transitions are resonant-limited and consequently QCC is established also in the domain  $v_{\text{RMT}} > 1$ . Obviously, at the same time we should satisfy the condition  $\tau_{cl} \ll t'_{\text{prt}}$ . It is easily verified that the latter condition cannot be satisfied if  $v_{\text{PR}} > 1$ . This is not just a technical limitation of the IMPT strategy, but reflects a real difference between two distinct routes towards QCC. This point is further illuminated in the next section.

### 17. Consequences of the IMPT treatment

The IMPT is capable of giving information about the tail, and hence about the second moment. Given  $t$ , one wonders how much  $b'$  can be ‘pushed down’ without violating the validity conditions of our procedure. It is quite clear that  $b' \gg b(t)$  is a necessary condition for *not* having a breakdown of perturbation theory. If we *assume* that the energy-spreading-profile is characterized just by the single parameter  $b(t)$ , then the condition  $b' \gg b(t)$  should be equivalent to  $t \ll t'_{\text{prt}}$ . Hence the following estimate is suggested:

$$b(t) = (t/\tau_c^{\text{qm}})^2 \quad (82)$$

We turn now to determine the  $\delta x_{\text{prt}}$  of the parametric evolution (PE), and then the  $t_{\text{prt}}$  of the actual evolution (AE). Recall that PE is obtained formally by ignoring the differences  $(E_n - E_m)$ , which implies that we can make in (80) the replacement  $\tilde{F}_t \mapsto t$ . Thus the tail of  $P(n|m)$  is band-limited and consequently the second moment is

$$s(t)^2 = b \times (1/\tau_c^{\text{qm}})^2 t^2 \quad [\text{band-limited tail}] \quad (83)$$

in agreement with the classical ballistic result (15). Our procedure for analyzing the core-tail structure of  $P(n|m)$  is meaningful as long as we have  $b(t) \ll s(t) \ll b$ . This defines an upper time limitation  $t_{\text{prt}}$  which is related via  $\delta x = Vt$  to the following parametric scale:

$$\delta x_{\text{prt}} = b^{1/2} \delta x_c^{\text{qm}} = \frac{\hbar}{\sqrt{\nu_{\text{E}} \tau_{cl}}} \quad (84)$$

At  $t = t_{\text{prt}}$  we have  $b(t) \sim s(t) \sim b$ , and we expect a crossover from a ballistic-like spreading to a genuine ballistic spreading.

In the perturbative regime the AE departs from the PE once the energy scale  $\Delta_b$  is resolved. This happens when  $t \sim \tau_{cl}$ . The perturbative approach is applicable for the analysis of the crossover at  $t \sim \tau_{cl}$  provided  $V\tau_{cl} \ll \delta x_{\text{prt}}$ . This is precisely the condition  $v_{\text{PR}} \ll 1$ . For  $t \gg \tau_{cl}$  the tail becomes resonance limited ( $|n-m| < (\hbar/t)/\Delta$ ) rather than band limited ( $|n-m| < b$ ) and we obtain:

$$s(t)^2 = (1/\tau_c^{\text{qm}})^2 t_{\text{H}} t \quad [\text{resonance-limited tail}] \quad (85)$$

in agreement with the classical diffusive result (16). Our procedure for analyzing the core-tail structure of  $P_t(n|m)$  is meaningful as long as we have  $b(t) \ll s(t) \ll b$ . This defines a *modified* upper time limitation

$$t_{\text{prt}} = (\tau_c^{\text{qm}})^{2/3} t_{\text{H}}^{1/3} = \left( \frac{\hbar^2}{\nu_{\text{E}} V^2} \right)^{1/3} \quad [\text{applies to } v_{\text{PR}} \ll 1] \quad (86)$$

At  $t = t_{\text{prt}}$  we have  $b(t) \sim s(t) \ll b$ , and we expect a crossover from a diffusive-like spreading to a genuine diffusive spreading.



## 18. Validity of the IMPT picture

It is important to have a clear understanding of the difference between the IMPT picture and the ORMT picture. In both cases we can argue that  $P(n|m)$  has, for short times, a core-tail structure. The fundamental difference is the assumption concerning the effective  $\tau_c$  for core-to-tail transitions. The ORMT picture assumes that effectively  $\tau_c = \tau_c^{\text{qm}}$ , and equivalently the tails grow like  $\delta x$ . This is the reason for having the premature crossover to diffusive growth (71) of the second moment. The IMPT picture assumes that the effective  $\tau_c$  is scale-dependent, and that the tails grow predominantly like  $\delta x^2$ . In other words, the tails grow as if we are still in the regime of FOPT. Therefore, from practical point of view, all we have to do in order to establish the validity of the IMPT picture is to verify that indeed the tails grow in a ballistic-like fashion ( $\propto \delta x^2$ ), and not in diffusive-like fashion ( $\propto \delta x$ ). A related observation is that also the core-width  $b(t)$  grows as ( $\propto \delta x^2$ ).

The argumentation (Sec. 16) in favor of the IMPT picture is not mathematically rigorous. It is therefore important to study specific examples. The obvious example to begin with has been defined by Wigner forty years ago [18, 20, 19]. Let  $\mathcal{H} = \mathbf{E} + x\mathbf{B}$  where  $\mathbf{E}$  is a diagonal matrix and  $\mathbf{B}$  is a banded random matrix. The IMPT picture should apply to the analysis of the PE of this Wigner model. Indeed, it is well known that  $P(n|m)$  for Wigner's model is a Lorentzian, and we may view this Lorentzian as a special case of core-tail structure. The width of the Wigner's Lorentzian, in energy units, is  $\Gamma = 2\pi((x \cdot \sigma)/\Delta)^2 \times \Delta$ . Thus we have indeed  $\propto \delta x^2$  for both the core and the tails. If the ORMT picture were true we would expect to get  $\propto \delta x$  dependence. All the results of the previous sections are consistent with the established results of Wigner. Having established the IMPT picture for PE, and observing that going from PE to AE involves no additional assumptions, it follows that we can safely proceed with the analysis as in Sec.17.

The validity of the the IMPT also has been verified numerically for the PE of the 'piston' example [15], and for the PE of a 2D nonlinear oscillator [16]. It has been verified that indeed the tails grow in a ballistic-like fashion ( $\propto \delta x^2$ ), and not in diffusive-like fashion ( $\propto \delta x$ ). Obviously, the assumption of having a structure-less *core* does not universally apply, and also having  $b(t) \propto \delta x^2$  is a quite fragile result. If we want to have a better idea about the core structure we should apply, in any special example, specific (non-perturbative) considerations. In case of the 'piston' example we can use semiclassical considerations [14] in order to argue that the core has a Lorentzian shape whose width is  $\hbar/\tau_{\text{col}}$ . This semiclassical Lorentzian has nothing to do with Wigner's Lorentzian. The semiclassical Lorentzian is a purely non-perturbative structure. This structure is exposed provided  $(\hbar/\tau_{\text{col}})/\Delta \ll b(t)$ , leading to the condition  $\delta x \gg \lambda_E$ . Else we have a structure-less core whose width is characterized by the single parameter  $b(t)$  of (82).

## 19. The quantum mechanical sudden approximation

It is now appropriate to discuss the QM sudden approximation. For the perturbative scenario ( $v_{\text{PR}} \ll 1$ ) we have already mentioned that the AE departs from the PE at  $t_{\text{sdn}} = \tau_{\text{cl}}$ , which is the time to resolve the energy scale  $\Delta_b$ . In case of the non-perturbative scenario ( $v_{\text{PR}} \gg 1$ ) there will be an *earlier breakdown* of the QM sudden approximation. This is because we have  $\tau_{\text{cl}} \gg t_{\text{prt}}$  and consequently at  $t = \tau_{\text{cl}}$  we already have  $s(t) \gg b$ . Therefore  $t_{\text{sdn}}$  should be defined as the time to resolve the energy scale which is associated with  $s(t)$ . It leads to

$$t_{\text{sdn}} = b^{1/4}(\tau_c^{\text{qm}}\tau_{\text{cl}})^{1/2} = \left(\frac{\hbar^2\tau_{\text{cl}}}{\nu_E V^2}\right)^{1/4} \quad \text{for } v_{\text{PR}} \gg 1 \quad (87)$$

perturbative route ( $v_{\text{PR}} \ll 1$ ):	
$t_{\text{sdn}} = \tau_{\text{cl}} \ll t_{\text{prt}}$	
At $t = \tau_{\text{cl}}$	$b(t) \ll s(t) \ll b \sim (\hbar/t)/\Delta$
At $t = t_{\text{prt}}$	$b(t) \sim s(t) \sim (\hbar/t)/\Delta \ll b$
Non-perturbative route ( $v_{\text{PR}} \gg 1$ ):	
$t_{\text{prt}} \ll t_{\text{sdn}} \ll \tau_{\text{cl}}$	
At $t = t_{\text{prt}}$	$b(t) \sim s(t) \sim b \ll (\hbar/t)/\Delta$
At $t = t_{\text{sdn}}$	$b \ll s(t) \sim (\hbar/t)/\Delta$
At $t = \tau_{\text{cl}}$	$b \sim (\hbar/t)/\Delta \ll s(t)$

**Table 4.** Various time scales in the route to stochastic behavior.

The various time scales are summarized in Table 4. The non-perturbative crossover from genuine-ballistic to genuine-diffusive behavior is not trivial. If  $v_{\text{SC}} \gg 1$  we can rely on semiclassical considerations in order to establish the existence of this crossover. More generally, for  $v_{\text{PR}} \gg 1$ , we would like to have an appropriate effective RMT model. This effective RMT model should support genuine-ballistic motion with an elastic scattering time  $\tau_{\text{cl}}$ .

## 20. The quantum mechanical adiabatic approximation

The previous analysis has emphasized the role of core-to-tail transitions in energy spreading. An implicit assumption was that these transitions are not suppressed by recurrences. This is not true in the QM adiabatic regime ( $v_{\text{LZ}} \ll 1$ ). Following [9] it is argued that energy spreading in the latter regime is dominated (eventually) by Landau-Zener transitions between near-neighbor levels. For completeness, the present section is devoted to the clarification of this observation.

As a preliminary exercise it is interesting to estimate the contribution of transitions between near-neighbor levels. The time scale that characterizes these transitions is  $\tau_c^{\text{qm}}$ , and the ‘step’ size is  $\Delta$ . Disregarding all other transitions, we have a random-walk process with diffusion coefficient  $(\Delta)^2/\tau_c^{\text{qm}}$ , leading to

$$D_{\text{E}}^{\text{NN}} \sim \frac{1}{v_{\text{LZ}}} D_{\text{E}}^{\text{cl}} \quad [\text{not applicable}] \quad (88)$$

Thus for  $v_{\text{LZ}} \gg 1$  the contribution of near-neighbor (NN) transitions is indeed negligible as expected. In the QM adiabatic regime ( $v_{\text{LZ}} \ll 1$ ) the above result should be modified as follows [9]:

$$D_{\text{E}}^{\text{LZ}} \approx \left( \frac{1}{v_{\text{LZ}}} \right)^{1-(\beta/2)} D_{\text{E}}^{\text{cl}} \quad \text{for } v_{\text{LZ}} \ll 1 \quad (89)$$

This result takes into account the non-trivial nature of Landau-Zener transitions and the statistics of the avoided-crossings. One should use  $\beta = 1$  for the Gaussian unitary ensemble (GUE) and  $\beta = 2$  for the Gaussian orthogonal ensemble (GOE). Recalling the stochastic considerations that lead to (88) one deduces that the perturbative breaktime is

$$t_{\text{prt}} = \left( \frac{1}{v_{\text{LZ}}} \right)^{\beta/2} \tau_c^{\text{qm}} \propto V^{-(1+(\beta/2))} \quad [\text{applies to } v_{\text{LZ}} \ll 1] \quad (90)$$

In the QM adiabatic regime energy spreading is dominated by near-neighbor level transitions for two distinct reasons. The first reason applies to the  $\beta = 1$  case, namely  $D_E^{\text{LZ}} \gg D_E^{\text{cl}}$ . The other reason is that  $D_E^{\text{cl}} \gg D_E^{\text{FGR}}$ . In the latter inequality,  $D_E^{\text{FGR}}$  is based on the FGR result (31). The FGR result becomes very small, compared with the classical result, once  $\bar{F}(\omega)$  becomes much narrower than the average level-spacing. The QM-adiabaticity condition  $t_{\text{H}} \ll \tau_c^{\text{qm}}$  means that individual energy levels are being resolved before the breakdown of first-order perturbation theory. Having no 'systematic' transitions to 'other' levels implies that the energy-distribution remains localized in the initial level for a very long time. The above argumentation implies that  $D_E^{\text{LZ}} \gg D_E^{\text{FGR}}$ , meaning that for extremely slow velocities energy spreading, and the eventual breakdown of the QM adiabatic approximation, is predominantly due to Landau-Zener mechanism.

## 21. Open questions and future directions

The purpose of this paper was to make the first steps towards a theory for energy spreading and quantum dissipation. In particular we wanted to demonstrate that perturbation theory, and semiclassical theory have different regimes of validity. There are still a lot of open questions that have to be answered.

An important issue is the specification of the general conditions for having a genuine stochastic behavior in the QM case. For fast velocities it is suggested (but not proved) that the stochastic behavior persists beyond the semiclassical brektime. For slow velocities, it is suggested (but again not proved) that the stochastic behavior persists beyond the brektime of perturbation theory. The latter suggestion is indirectly supported by common-wisdom and by various numerical experiments with banded matrices [26, 10, 24]. For the generic RMT picture, which is still lacking, it is implied that both, breakdown of perturbation theory and resolving the bandwidth of first-order transitions, are necessary conditions for having genuine stochastic behavior. In any case, stochasticity *can be established* if we assume irregular a-periodic driving with an appropriate correlation scale. For periodic driving, further considerations are required in order to analyze the possible manifestation of localization effect.

A better understanding of the core-tail structure is required. Only in the case of Wigner's model [18, 19, 20] we have an established result: Namely, the core-tail structure is simply a Lorentzian. For real systems the core-tail structure is not necessarily a Lorentzian [14]. The determination of the border between the core and the tail may be problematic. One cannot exclude the existence of a distinct tail component, in the vicinity of the core, that does not grow like  $\delta x^2$ . A strongly related issue is to get an analytical understanding of the  $b'$  dependence of the effective ('renormalized') correlation time  $\tau_c$ .

The 'piston' example is non-generic in many respects. There are three classical length scales: The penetration distance upon collision with the piston; The mean path-length between collisions with the piston; And the ballistic length scale that characterizes the volume of the cavity. Quantum-mechanics adds two additional length scales: one is related to the Airy structure in the vicinity of the turning points, and the other is the De-Broglie wavelength. Having all these scales has some non-universal consequences [14] that we have not considered in this paper. The application of the general theory of sections 8-20 to the 'piston' example is quite straightforward, but these non-universal features should be taken into account. In the generic theory there are only two parametric scales: The displacement  $\delta x_c^{\text{qm}}$  that is needed in order to mix neighboring levels; And the displacement  $\delta x_{\text{prt}}$  that is needed in order to mix the core with the tail. The former is much smaller than De-Broglie wavelength, and the latter is much larger than De-Broglie wavelength. It turns out that in the 'piston'

example there is a third, non-universal parametric scale  $\delta x_{\text{NU}}$  that roughly equals to De-Broglie wavelength [14]. Consequently, the perturbative (slow-velocity) regime is further divided into a universal slow-velocity regime, and a non-universal slow-velocity regime.

Of particular importance is the understanding of the *hard-wall limit*. In the generic theory  $\tau_{\text{cl}}$  determines the bandwidth  $\Delta_b$  of the matrix  $\mathbf{W}_{nm}$ . Having *finite bandwidth* is essential in order to understand that there is a crossover to a *non-perturbative* regime in the  $\hbar \rightarrow 0$  limit. We cannot treat  $\mathbf{W}_{nm}$  as a banded matrix if we take first the limit  $\tau_{\text{cl}} \rightarrow 0$ . The walls of the ‘piston’ should be regarded as ‘hard’ once  $\Delta_b$  becomes equal or larger than  $E$ . This is equivalent to having (classical) penetration distance smaller than De-Broglie wavelength. The consequence of taking the hard wall limit is that the non-perturbative regime ( $v_{\text{PR}} > 1$ ) disappears. This state-of-affairs is possibly responsible to the *illusion* that a *general* theory for quantum dissipation can be base on a perturbative approach. At first sight it looks strange that hard-walls are ‘better’ for perturbation theory. It looks even more strange that for hard walls we cannot apply the semiclassical theory. In order to make the latter observation less strange recall that solving the one-dimensional Schroedinger equation near a sharp step, and then taking  $\hbar \rightarrow 0$ , never corresponds to the WKB approximation.

The problem of quantum dissipation, in the sense of this paper, is a preliminary stage in the construction of a theory [34] of quantal Brownian motion (QBM). In the classical case it is known [11] that the motion of a ‘heavy’ particle that is coupled to *chaotic* degrees-of-freedom is quite generally described by the classical Langevin equation. The effect of the environment is represented by a friction force plus a noise term. The friction leads to dissipation of energy and the noise term is essential for having diffusion. Furthermore, the friction coefficient is related to the noise intensity via the universal  $\mathcal{FD}$  relation. The fact that there is no general theory for quantum dissipation, and a-fortiori there is no general theory of QBM, has not been universally recognized in the literature. It is true that there is a vast literature that comes under those headings, but actually this literature is commonly based on an *effective-bath approach*. In previous studies [27, 28, 29] the common effective-bath strategy has been applied in order to develop a universal description of QBM and dephasing. Another possibility is to use an effective RMT bath [30]. The results of the latter study agree with [27, 28]. A future theory of QBM should clarify whether effective-bath methods universally apply.

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### Appendix A. The sudden and the adiabatic approximations

For the time dependent Hamiltonian  $\mathcal{H}(Q, P; x(t))$  energy is not a constant of the motion. Changes in the actual energy  $\mathcal{E}(t)$  reflect ‘real’ dynamical changes as well as parametric changes. Therefore it is useful to introduce the following definitions:

$$\mathcal{E}(t) = \mathcal{H}(Q(t), P(t); x(t)) \quad (\text{A.1})$$

$$\mathcal{E}'(t) = \mathcal{H}(Q(t), P(t); x(0)) \quad (\text{A.2})$$

For simplicity we assume that the phase space volume  $\Omega(E; x)$  is independent of  $x$ , thus  $F(x) = 0$ . The actual energy change can be calculated as follows:

$$\delta\mathcal{E} = \mathcal{E}(t) - \mathcal{E}(0) = -V \int_0^t \mathcal{F}(t') dt' \quad (\text{A.3})$$

The actual energy change  $\delta\mathcal{E}$  can be viewed as a sum of parametric-energy-change  $\delta\mathcal{E}_o$ , and reduced-energy-change  $\delta\mathcal{E}'$ .

$$\delta\mathcal{E} = \mathcal{H}(Q(t), P(t); x(t)) - \mathcal{H}(Q(0), P(0); x(0))$$

$$\delta\mathcal{E}_o = \mathcal{H}(Q(t), P(t); x(t)) - \mathcal{H}(Q(t), P(t); x(0))$$

$$\delta\mathcal{E}' = \mathcal{H}(Q(t), P(t); x(0)) - \mathcal{H}(Q(0), P(0); x(0))$$

The reduced energy change  $\delta\mathcal{E}'$  reflects the deviation of  $(Q, P)$  from the original energy surface. It can be calculated as follows:

$$\delta\mathcal{E}' = V \cdot \left[ \mathcal{F}(t) \times t - \int_0^t \mathcal{F}(t') dt' \right] \quad (\text{A.4})$$

On the other hand, the actual energy change  $\delta\mathcal{E}$  reflects the deviation of  $(Q, P)$  from the instantaneous energy surface.

By inspection of the expressions for the reduced energy change we arrive at the conclusion that for short times we have the so called ‘sudden approximation’:

$$\delta\mathcal{E}' \approx 0 \quad \text{for } t \ll \tau_{cl} \quad (\text{A.5})$$

By inspection of the expression for the actual energy change we arrive at the conclusion that for long times we have the so called ‘adiabatic approximation’:

$$\delta\mathcal{E} \sim 0 \quad \text{for } t \ll t_{\text{fre}} \quad (\text{A.6})$$

The time evolution of an initially localized phase-space distribution  $\rho_0(Q, P)$  is illustrated in Fig.2. For short times we have in general non-stationary time evolution:

$$\mathcal{U}(t) \rho_0(Q, P) \neq \rho_0(Q, P) \quad \text{for } t \ll \tau_{cl}$$

Here  $\mathcal{U}(t)$  is the classical propagator of phase space points. However, if we operate with the same  $\mathcal{U}(t)$  on a microcanonical distribution, then

$$\mathcal{U}(t) \rho_{E,x(0)}(Q, P) \approx \rho_{E,x(0)}(Q, P) \quad \text{for } t \ll \tau_{cl}$$

Thus, the sudden approximation implies that for short times  $\mathcal{U}(t)$  can be replaced by *unity* if it operates on an initial microcanonical distribution. For long times we have

$$\mathcal{U}(t) \rho_0(Q, P) \sim \rho_{E,x(t)}(Q, P) \quad \text{for } t_{\text{erg}} \ll t \ll t_{\text{fre}}$$

It is not required to start with a microcanonical distribution, unless  $\tau_{cl} \ll t \ll t_{\text{erg}}$ . The adiabatic approximation becomes worse and worse as time elapse due to the transverse spreading across the energy surface.  $t_{\text{fre}}$  is the brektime of the adiabatic approximation. See discussion after (43).

## Appendix B. The conventional FGR Picture

The simplest version of time-dependent perturbation theory is based on the approximated Hamiltonian

$$\mathcal{H}(Q, P; x(t)) \approx \mathcal{H}(Q, P; x(0)) + \frac{\partial \mathcal{H}}{\partial x} x(t) \quad (\text{B.1})$$

and using a *fixed basis* that is determined by the unperturbed Hamiltonian  $\mathcal{H}(Q, P; x(0))$ . For simplicity we set  $x(0)=0$ . A limitation that follows from using fixed basis is that the crossover from ballistic to diffusive spreading is out-of-reach for this version of perturbation theory.

Another limitation of the present FGR picture stems from the fact that some additional assumptions should be imposed on  $x(t)$ , else the treatment may be not valid. We shall assume that at any time  $x(t) \ll \delta x_c^{\text{cl}}$ , so that the expansion in (B.1) is valid. Moreover we shall assume that  $x$  is being changed in an arbitrary a-periodic fashion, such that  $\dot{x}(t)$  becomes uncorrelated on a time scale  $\tau_c^{\text{drv}}$ . The assumption  $\tau_{\text{cl}} \ll \tau_c^{\text{drv}}$  is implied by the trivial definition of slowness (11). The loss of velocity-velocity correlation will be described by a function  $F(\tau)$ , with the convention  $F(0) = 1$ . This function should satisfy the normalization  $\int F(\tau) d\tau = 0$ , else we will have an unbounded growth of  $(x(t) - x(0))^2$ . We still assume that the typical ‘velocity’ is  $V$ , meaning that  $\langle \dot{x}(t) \dot{x}(t+\tau) \rangle = V^2 F(\tau)$ . The above assumptions implies that the correlator  $\langle x(t)x(t+\tau) \rangle = F(\tau)$  is well defined. Its Fourier transform satisfies  $\tilde{F}(\omega) = V^2 \tilde{F}(\omega)/\omega^2$ . Note that the normalization of the frequency distribution  $\tilde{F}(\omega)$  is 1, while the normalization of  $\tilde{F}(\omega)$  is  $(V\tau_c^{\text{drv}})^2$ .

The FGR expression for the transition rate from the energy levels  $m$  to some other energy level  $n$  is:

$$\Gamma_{nm} = \frac{1}{\hbar^2} \left| \left( \frac{\partial \mathcal{H}}{\partial x} \right)_{nm} \right|^2 \tilde{F} \left( \frac{E_n - E_m}{\hbar} \right) \quad (\text{B.2})$$

From here follows an expression for the diffusion constant. This expression is easily cast into a classical look-alike formula:

$$D_{\text{E}} = \frac{1}{2} \frac{1}{\mathcal{N}} \sum_{nm} \Gamma_{nm} (E_n - E_m)^2 = \frac{1}{2} V^2 \int_{-\infty}^{\infty} C_{\text{E}}(\tau) F(\tau) d\tau \quad (\text{B.3})$$

It is argued that (B.2) is valid for any  $t > \tau_c^{\text{drv}}$  provided there is a separation of time scales  $\tau_c^{\text{drv}} \ll \tau_{\text{prt}}$ . This is the ‘golden-rule’ condition, namely, breaktime of first-order perturbation theory should be after  $\tau_c^{\text{drv}}$ . We use the notation  $\tau_{\text{prt}}$  rather than  $t_{\text{prt}}$  in order to emphasize that fixed-basis perturbation theory is being used. The persistence of transitions with the *same* rate for  $t > \tau_{\text{prt}}$  is guaranteed due the stochastic nature of the dynamics: The irregular driving is like noise, and interference contribution is averaged to zero once time intervals larger than  $\tau_c^{\text{drv}}$  are being composed. Let us assume further that  $\tau_{\text{prt}} \ll t_{\text{H}}$ , in order to guarantee that there are no recurrences irrespective of  $\tau_c^{\text{drv}}$ . Gathering all our assumption together (classical slowness condition, FGR condition, and the non-recurrence condition) we get:

$$\tau_{\text{cl}} \ll \tau_c^{\text{drv}} \ll \tau_{\text{prt}} \ll t_{\text{H}} \quad (\text{B.4})$$

It should be noted that the classical slowness condition implies resonance-limited transitions and hence restricted QCC is guaranteed.

We turn now to get an actual estimate for the perturbative breaktime  $\tau_{\text{prt}}$ , and for the associated slowness condition. The total transition rate from a level  $m$  is  $\Gamma = \sum'_n \Gamma_{nm}$ , and we have

$$\tau_{\text{prt}} = \frac{1}{\Gamma} = \frac{\hbar^2}{\nu_{\text{E}} V^2 (\tau_c^{\text{drv}})^2} \quad \text{fixed-basis, } \nu_{\text{PR}} \ll 1 \quad (\text{B.5})$$

The maximal value of  $\tau_{\text{prt}}$  is attained if  $\tau_c^{\text{drv}} = \tau_{\text{cl}}$ . The minimal value  $\tau_{\text{prt}} = t_{\text{prt}}$  is attained for  $\tau_c^{\text{drv}} = t_{\text{prt}}$ . One easily concludes that a necessary condition for the applicability of the FGR picture is

$$V \ll \frac{\hbar/\tau_{\text{cl}}}{\sqrt{\nu_E \tau_{\text{cl}}}} \quad \text{QM definition of slowness} \quad (\text{B.6})$$

The latter condition is always violated in the classical limit. Thus, it is *not possible in principle* to establish QCC in the limit  $\hbar \rightarrow 0$  by using FGR picture. Note that (B.6) is equivalent to (23) leading to  $v_{\text{PR}} \ll 1$ .

### Appendix C. Alternative derivation of the ‘sudden time’

Simple considerations based on fixed-basis perturbation theory can be used in order to derive a result for  $t_{\text{sdn}}$ . By ‘sudden approximation’ we mean that for a limited time we can ‘ignore’ the dynamical changes that are generated by the Hamiltonian. A necessary condition is that the transition probability between levels is much less than unity, or equivalently  $t \ll \tau_{\text{prt}}$ . It is essential to use the breaktime  $\tau_{\text{prt}}$  of *fixed-basis* perturbation theory, since we want to avoid the fake transitions due to non-trivial parametric-evolution. However,  $t \ll \tau_{\text{prt}}$  is not a sufficient condition. If  $|\psi\rangle$  is a superposition of few levels, then we should also require that the corresponding energies will not be resolved. Namely we should have  $|E_n - E_m|t \ll \hbar$  for any  $n$  and  $m$  in the superposition. We are interested in the way in which energy is re-distributed. Therefore, as long as first order perturbation theory applies, it is not important whether energy levels are resolved unless they are directly coupled ( $|E_n - E_m| < \Delta_b$ ). It follows that

$$t_{\text{sdn}} = \text{minimum}(\tau_{\text{prt}}, \tau_{\text{cl}}) \quad (\text{C.1})$$

where  $\tau_{\text{prt}}$  is the breaktime of fixed-basis perturbation theory. It is a trivial matter to estimate the transition probabilities. Since we are interested in short times ( $t < \tau_{\text{cl}} < \tau_c^{\text{drv}}$ ) we can substitute  $x(t) = Vt$  in (B.1), and we get:

$$\text{transition probability} = \left| \frac{1}{2} \frac{1}{\hbar} \left( \frac{\partial \mathcal{H}}{\partial x} \right)_{nm} V t^2 \right|^2 \quad \text{for } n \neq m \quad (\text{C.2})$$

Note that the FGR expression for the transition probability, namely  $\Gamma_{nm}t$ , is valid in a different time regime ( $t \gg \tau_c^{\text{drv}} \gg \tau_{\text{cl}}$ ). The transition-probability to each of the levels within the band is approximately the same, and upon multiplication by  $b$ , an expression for the total transition-probability is easily obtained. It can be written as  $(t/\tau_{\text{prt}})^4$  where

$$\tau_{\text{prt}} = \left( \frac{\hbar^2 \tau_{\text{cl}}}{\nu_E V^2} \right)^{1/4} \quad \text{fixed-basis, } v_{\text{PR}} \gg 1 \quad (\text{C.3})$$

If the velocity  $V$  is not slow (in the sense of (B.6)), then we have  $t_{\text{sdn}} = \tau_{\text{prt}} < \tau_{\text{cl}}$ . For slow velocities we have  $\tau_{\text{prt}} \gg \tau_{\text{cl}}$  and therefore  $t_{\text{sdn}} = \tau_{\text{cl}}$ . In the latter case expression (C.3) underestimates the perturbative breaktime: Once  $t \gg \tau_{\text{cl}}$  the transitions become resonance-limited, and consequently a diffusive-like spreading develops. Thus, in the slow velocity regime the FGR expression (B.5) for the perturbative breaktime  $\tau_{\text{prt}}$  should be used. Taking into account the restrictions on  $\tau_c^{\text{drv}}$  one observes that going from (C.3) to (B.5) does not involve any discontinuity.

### Appendix D. Spherical coordinates and related results

The solid angle in  $d$  dimension and the volume element in spherical coordinates are

$$\Omega_d = \frac{2\pi^{d/2}}{\Gamma(d/2)} = 2, 2\pi, 4\pi, \dots \quad (\text{D.1})$$

$$d\Omega_d r^{d-1} dr = d\Omega_{d-1} (\sin(\theta))^{d-2} d\theta r^{d-1} dr \quad (\text{D.2})$$

The following results are easily derived:

$$\langle |\cos(\theta)| \rangle = \frac{1}{\sqrt{\pi}} \frac{\Gamma(d/2)}{\Gamma((d+1)/2)} = 1, \frac{2}{\pi}, \frac{1}{2}, \dots \quad (\text{D.3})$$

$$\langle |\cos(\theta)|^3 \rangle = \frac{1}{\sqrt{\pi}} \frac{\Gamma(d/2)}{\Gamma((d+3)/2)} = 1, \frac{4}{3\pi}, \frac{1}{4}, \dots \quad (\text{D.4})$$

Note the relation  $2\langle |\cos(\theta)| \rangle = (d+1)\langle |\cos(\theta)|^3 \rangle$ .

It is useful to define a generalized cosine function by averaging  $\exp(i\mathbf{n}\cdot\mathbf{r})$  over the orientation of the unit vector  $\mathbf{n}$ . The averaging is easily performed by using spherical coordinates:

$$\text{Cos}(r) = \langle e^{ir \cos(\theta)} \rangle = 2^{\frac{d}{2}-1} \Gamma(\frac{d}{2}) \frac{J_{\frac{d}{2}-1}(r)}{r^{\frac{d}{2}-1}} \quad (\text{D.5})$$

It is also useful to define a generalized sinc function as follows:

$$\text{Sinc}(r) = -\frac{\text{Cos}'(r)}{r} = \frac{1}{d} 2^{\frac{d}{2}} \Gamma(\frac{d}{2}+1) \frac{J_{\frac{d}{2}}(r)}{r^{\frac{d}{2}}} \quad (\text{D.6})$$

The function  $(\text{Sinc})^2$  will appear in an integral over a  $(d-1)$  dimensional surface. It will be possible to replace it by an effective delta-function:

$$(\text{Sinc}(k|\mathbf{s}_2 - \mathbf{s}_1|))^2 \longrightarrow \left(\frac{2\pi}{k}\right)^{d-1} \frac{2\langle |\cos(\theta)|^3 \rangle}{\Omega_d} \delta(\mathbf{s}_2 - \mathbf{s}_1) \quad (\text{D.7})$$

In order to derive this result one should use the following:

$$\int_0^\infty \frac{(J_\nu(x))^2}{x^2} dx = \frac{4}{\pi(4\nu^2-1)} \quad (\text{D.8})$$

$$\int_0^\infty (\text{Sinc}(r))^2 \Omega_{d-1} r^{d-2} dr = \frac{\Omega_{d-1}}{\pi} \frac{2^d}{d^2-1} (\Gamma(\frac{d}{2}))^2 \quad (\text{D.9})$$



### Appendix E. Collisions with a wall: phase space approach

The position of a particle inside a cavity can be described by  $Q = (z, \mathbf{x}_\perp)$  where  $z$  is perpendicular to the surface. The potential which is experienced by the particle is assumed to be  $\mathcal{V}(Q) = 0$  inside the cavity where  $z < 0$ , and  $\mathcal{V}(Q) = f \cdot z$  for  $z > 0$ . Let the variable  $x$  parameterize the perpendicular displacement of the surface (hence  $\mathbf{n} \cdot \mathbf{V} = 1$ ). With this parameterization we have simply  $\mathcal{F}(Q, P; x) = f$  provided  $z > 0$ , else  $\mathcal{F}(Q, P; x) = 0$ . For an isolated collision we have

$$z(t \pm \frac{1}{2}\tau) = z \pm \frac{p_z}{m} \cdot (\frac{1}{2}\tau) - \frac{1}{2} \frac{f}{m} (\frac{1}{2}\tau)^2 \quad (\text{E.1})$$

The correlation function is

$$C_E(\tau) = \frac{f^2 \int d\mathbf{p}_\perp \int dp_z \int d\mathbf{x}_\perp \int dz \delta\left(E - \left(\frac{\mathbf{p}^2}{2m} + f \cdot z\right)\right)}{\int d\mathbf{p} \int d\mathbf{x} \delta\left(E - \frac{\mathbf{p}^2}{2m}\right)} \quad (\text{E.2})$$

The integration in the numerator is restricted by the conditions  $z(t + \frac{1}{2}\tau) > 0$  and  $z(t - \frac{1}{2}\tau) > 0$ . The  $d\mathbf{x}_\perp$  integration gives an *Area* factor. After the  $dz$  integration one is left with a  $d\mathbf{p}$  integration that represents the volume  $\mathbf{p}^2 + 2(\frac{1}{2}f\tau)p_z + (\frac{1}{2}f\tau)^2 < 2mE$ . Using spherical coordinates one obtains

$$C_E(\tau) = \frac{\text{Area} \cdot f \cdot 2 \int \Omega_{d-1} (\sin \theta)^{d-2} d\theta \int p^{d-1} dp}{\text{Volume} \cdot \frac{1}{2} \Omega_d ((2mE)^{1/2})^d / E} \equiv \nu_E \hat{C}_E\left(\frac{\tau}{\tau_{e1}}\right)$$

The  $d\theta$  and the  $dp$  integrations in the numerator are restricted by the conditions  $(\frac{1}{2}f\tau)/(2mE)^{1/2} < \cos \theta < 1$  and  $(\frac{1}{2}f\tau)/\cos \theta < p < (2mE)^{1/2}$  respectively. The noise intensity is

$$\nu_E = 2 \langle |\cos \theta|^3 \rangle \frac{\text{Area}}{\text{Volume}} m^2 v_E^3 \quad (\text{E.3})$$

The properly normalized  $\hat{C}_E(\tau)$  equals zero for  $|\tau| > 1$  and otherwise can be expressed using an hypergeometrical function as follows:

$$\begin{aligned} \hat{C}_E(\tau) &= \frac{d^2-1}{2d} \int_{\tau < \cos \theta} (\sin \theta)^{d-2} d\theta \left[ 1 - \left( \frac{|\tau|}{\cos \theta} \right)^d \right] \\ &= \frac{d+1}{2d} \left( \frac{1}{\tau^2} - 1 \right)^{\frac{d-1}{2}} \left[ {}_2F_1 \left( \frac{d-1}{2}, \frac{d}{2}; \frac{d+1}{2}; - \left( \frac{1}{\tau^2} - 1 \right) \right) - |\tau|^d \right] \\ &= \begin{cases} \frac{3}{4} \left( \arctan \left( \sqrt{\frac{1}{\tau^2} - 1} \right) - \tau^2 \sqrt{\frac{1}{\tau^2} - 1} \right) & \text{for } d = 2 \\ \frac{2}{3} (|\tau|^3 - 3|\tau| + 2) & \text{for } d = 3 \end{cases} \end{aligned} \quad (\text{E.4})$$

It is much easier to obtain an explicit expression for  $C_T(\tau)$ . The  $\delta(\text{energy})$  function in (E.2) should be replaced by  $\exp(-\text{energy}/(k_B T))$ . The integration is factorized, and one obtains

$$C_T(\tau) = \frac{\text{Area}}{\text{Volume}} k_B T f \cdot \text{erfc} \left( \frac{1}{2} \frac{f}{\sqrt{2m k_B T}} |\tau| \right) \quad (\text{E.5})$$

The noise intensity  $\nu_T$  can be found either by integration over this function, or else by performing thermal average over  $\nu_E$ . In both cases the result is:

$$\nu_T = \frac{4}{\sqrt{\pi}} \frac{\text{Area}}{\text{Volume}} k_B T (2m k_B T)^{1/2} \quad (\text{E.6})$$

### Appendix F. Collisions with a wall: time domain approach

Consider the motion of a particle inside a chaotic cavity. we can define and estimate the collision rate with a wall element as follows:

$$\frac{1}{\tau_{\text{col}}} = \left\langle \sum_{\text{col}} \delta(t - t_{\text{col}}) \right\rangle = \frac{1}{2} \frac{ds}{\text{Volume}} \langle |\cos \theta| \rangle v_E \quad (\text{F.1})$$

Above  $t_{\text{col}}$  is the time of of a collision, and  $ds$  is the area of the wall element. The derivation of last equality is based on ergodicity considerations which we are going to explain now. Let us define the coordinate  $z$  as in the previous appendix. We have

$$\delta(z(t)) = \sum_{\text{col}} \sum_{\pm} \frac{1}{|(v_z)_{\text{col}}|} \delta(t - t_{\text{col}}^{\pm}) = \sum_{\text{col}} \frac{2}{v_E |\cos \theta_{\text{col}}|} \delta(t - t_{\text{col}})$$

where  $t_{\text{col}}^{\pm}$  correspond to the crossing times of the  $z = 0$  surface, and  $t_{\text{col}} = (t_{\text{col}}^+ + t_{\text{col}}^-)/2$  is the time of the collision. The duration of the collision  $\Delta t_{\text{col}} = (t_{\text{col}}^+ - t_{\text{col}}^-)$  is assumed to be extremely short. Equivalently we can write  $\sum \delta(t - t_{\text{col}}) = \frac{1}{2} v_E |\cos \theta| \delta(z(t))$ . In order to get (F.1), the latter expression should be averaged over the (implicit) initial conditions  $(Q(0), P(0))$ . As always  $\langle \dots \rangle$  indicates this type of averaging. Due to the chaos, the coordinate  $z$  and  $\cos \theta$  can be treated as independent variables. Due to ergodicity we have  $\langle \delta(z(t)) \rangle = \langle \delta(z) \rangle_E = ds/\text{Volume}$ . As always  $\langle \dots \rangle_E$  stands for a microcanonical average. For  $\langle |\cos \theta| \rangle$  one may substitute (D.3).

Exactly the same procedure can be used in order to estimate  $\nu_E$ . The first step is to realize that  $\partial \mathcal{H}/\partial x = (\mathbf{n} \cdot \hat{\mathbf{V}}) \times f$  for  $z > 0$ , and *zero* otherwise. The fluctuating force  $\mathcal{F}(t) = -\partial \mathcal{H}/\partial x$  looks like a train of short impulses. The duration of each impulse is  $\Delta t_{\text{col}} = 2m|(v_z)_{\text{col}}|/f$ . Therefore we can write

$$\mathcal{F}(t) = -\frac{\partial \mathcal{H}}{\partial x} = \sum_{\text{col}} [ (\mathbf{n} \cdot \hat{\mathbf{V}}) 2mv_E \cos(\theta_{\text{col}}) ] \delta(t - t_{\text{col}}) \quad (\text{F.2})$$

The intensity of the fluctuations due to this random-like sequence of delta-impulses is

$$\nu_E = \left\langle \sum_{\text{col}} [ (\mathbf{n} \cdot \hat{\mathbf{V}}) 2mv_E \cos(\theta_{\text{col}}) ]^2 \delta(t - t_{\text{col}}) \right\rangle$$

The last expression is manipulated as in (F.1) and leads to the correct result.

It is more illuminating to repeat the last derivation using a kinetic point of view. The velocity of the particle prior to the collision with the wall element is  $\mathbf{v}_{\text{col}}$ . The orientation of the wall element is represented by a normal unit vector  $\mathbf{n}$ . The velocity of the wall element is denoted by  $\mathbf{V}$ . Only the  $\mathbf{n} \cdot \mathbf{V}$  component of the wall velocity is significant. After the collision the  $z$  component of the particle's velocity is  $\mathbf{n} \cdot (-\mathbf{v}_{\text{col}} + 2\mathbf{V})$ . The corresponding energy gain due to the collision is

$$\Delta E_{\text{col}} = -2m (\mathbf{n} \cdot \mathbf{V}) (\mathbf{n} \cdot (\mathbf{v}_{\text{col}} - \mathbf{V})) \quad . \quad (\text{F.3})$$

The stochastic-like force  $\mathcal{F}(t)$  is a sum over impulses that are created by collisions with the surface of the cavity. The energy gain due to this collisions is obtained by integrating  $-V\mathcal{F}(t)$  over time (see Sec.4). It follows that each collision involves an impulse  $-\Delta E_{\text{col}}/V$  leading to

$$\mathcal{F}(t) = \sum_{\text{col}} [ 2m (\mathbf{n} \cdot \hat{\mathbf{V}}) (\mathbf{n} \cdot (\mathbf{v}_{\text{col}} - \mathbf{V})) ] \delta(t - t_{\text{col}}) \quad (\text{F.4})$$

For  $V=0$  we can assume that the velocities  $v_{\text{col}}$  are uncorrelated. For a moving slab-shaped 'piston' half of the collisions will be from the 'left side' with  $\mathbf{n} \cdot \mathbf{V} = -V$ , and half of the collisions will be from the 'right' side with  $\mathbf{n} \cdot \mathbf{V} = +V$ . Consequently we have  $\langle \mathcal{F}(t) \rangle = 0$ . More generally, we have  $\langle \mathcal{F}(t) \rangle = 0$  for any parametric deformation that keeps constant the total volume of the cavity.

It is now tempting to make an attempt for a direct estimate of  $\langle \mathcal{F}(t) \rangle$  for  $V \neq 0$ . Let us assume for a moment that we have a slab-shaped ‘piston’ which is moving from ‘left’ to ‘right’. At first sight it seems that friction is due to the fact that energy-gain due to collisions from the ‘right’ is larger than energy-loss due to collisions from the ‘left’. Our “hypothesis” implies that the  $\mathcal{O}(V)$  term in (F.4) should be responsible for the friction. However, it turns out that only *half* of the correct result is obtained:

$$\left\langle \sum_{\text{col}} 2m(\mathbf{n} \cdot \hat{\mathbf{V}})^2 \delta(t-t_{\text{col}}) \right\rangle = \langle |\cos \theta| \rangle \frac{\text{Area}}{\text{Volume}} m v_{\text{E}} = \frac{1}{2} \mu_{\text{E}}$$

We conclude that the first term in (F.4), the term that includes  $v_{\text{col}}$ , has a non-zero average. Once  $V \neq 0$  we can no-longer treat the collisions as uncorrelated. The statistical effect (that has been emphasized in the derivation of the  $\mathcal{FD}$  relation) is important also in time-domain analysis.

Thus we see that the  $\mathcal{FD}$  indirect approach is a quite powerful tool. This becomes manifestly evident once we consider a variation of the above example: If successive collisions with the ‘piston’ are correlated, for example due to bouncing behavior, then it is still a relatively easy task to estimate  $\nu_{\text{E}}$  for the  $V=0$  case, and then to obtain  $\mu_{\text{E}}$  via the  $\mathcal{FD}$  relation. On the other hand, a direct evaluation of  $\mu_{\text{E}}$  using kinetic considerations is extremely difficult, because in calculating  $\langle \mathcal{F}(t) \rangle$  it is essential to take into account subtle correlations between successive collisions.

### Appendix G. The wall formula: the standard kinetic approach

Here we generalize the derivation of the wall formula to any dimension, and to any dispersion relation  $E = E(\mathbf{p})$ . We use the standard kinetic approach. The momentum probability distribution of the particles inside the cavity is uniform in space and  $\rho(\mathbf{p})$  in momentum. (Later we are using many-particles jargon, but the actual meaning is always probabilistic). We assume isotropic distribution, and therefore the energy distribution is just  $\rho(E) = g(E)\rho(p)$ . The velocity which is associated with a momentum  $\mathbf{p}$  is  $\mathbf{v}=dE/d\mathbf{p}$ . The mass is defined in the differential sense  $m(E) = (dv/dp)^{-1}$ .

With a surface area  $ds$  we associate a normal unit vector  $\mathbf{n}$ , and a displacement velocity  $\mathbf{V}$ . The particles that actually collide with the wall-element during a time interval  $dt$  must satisfy the condition  $(\mathbf{v}-\mathbf{V}) \cdot \mathbf{n} > 0$ . Those with a velocity  $\mathbf{v}$  are contained in a volume element  $d\text{Volume} = ((\mathbf{v}-\mathbf{V}) \cdot \mathbf{n}) dt ds$ . The energy gain due to a collision, assuming  $V \ll v$ , and expanding up to  $\mathcal{O}(V^2)$ , is still given by (F.3). The total energy change is

$$dE = \int \rho(\mathbf{p}) d\mathbf{p} \times d\text{Volume} \times \Delta E_{\text{col}} \quad (\text{G.1})$$

The above integral can be manipulated as follows: We make a transformation to an integration variable  $\mathbf{p}' = \mathbf{p} - m\mathbf{V}$  and correspondingly  $\mathbf{v}' = \mathbf{v} - \mathbf{V}$ . Then we expand  $\rho(\mathbf{p}'+m\mathbf{V}) = \rho(\mathbf{p}') + (\partial\rho(p')/\partial E)m\mathbf{v}' \cdot \mathbf{V}$ , and throw away the first term since it is associated with reversible work. From here on we omit the primes. Due to symmetry consideration we may replace  $\mathbf{v} \cdot \mathbf{V}$  by  $(\mathbf{v} \cdot \mathbf{n})(\mathbf{V} \cdot \mathbf{n})$ . Now we obtain

$$dE = - \int \frac{\partial\rho(p)}{\partial E} d\mathbf{p} m^2 (\mathbf{V} \cdot \mathbf{n})^2 |\mathbf{v} \cdot \mathbf{n}|^3 ds dt \quad (\text{G.2})$$

The latter integral is easily cast into the form of (19) with the identification

$$D_{\text{E}} = \frac{\langle |\cos(\theta)|^3 \rangle}{\text{Volume}} m^2 v_{\text{E}}^3 \oint (\mathbf{V} \cdot \mathbf{n})^2 ds \quad (\text{G.3})$$

The latter expression incorporates integration over all the wall-elements.

## Appendix H. Chaotic eigenstates

The average density of energy eigenstates for a particle in  $d$  dimensional cavity is

$$\frac{1}{\Delta} = \frac{1}{\hbar v_E} \frac{\text{Volume}}{(2\pi)^d} \Omega_d k^{d-1} \quad (\text{H.1})$$

where  $k$  is the wavenumber and  $v_E$  is the corresponding velocity of the particle. An eigenstate that corresponds to a chaotic cavity looks like a ‘random wave’. More precisely, it has the same statistical properties as those of an un-constrained random superposition of plane waves whose wavenumber is  $|\mathbf{k}| = k$ . It is characterized by the correlation function

$$\langle \psi_R(\mathbf{x}_1) \psi_R(\mathbf{x}_2) \rangle = \frac{1}{\text{Volume}} \text{Cos}(k|\mathbf{x}_2 - \mathbf{x}_1|) \quad (\text{H.2})$$

The function Cos is defined in App.Appendix D. We can constrain a random wave to be zero along a boundary by making an antisymmetric superposition of an un-constrained random wave with its mirror image. The normal derivative along the boundary  $\varphi(\mathbf{s}) = \mathbf{n} \cdot \nabla \psi$  satisfies

$$\langle \varphi_R(\mathbf{s}_1) \varphi_R(\mathbf{s}_2) \rangle = \frac{2k^2}{\text{Volume}} \text{Sinc}(k|\mathbf{s}_2 - \mathbf{s}_1|) \quad (\text{H.3})$$

This expression ignores curvature effect. We assume that the boundary’s radius-of-curvature is very large compared with De-Broglie wavelength, as well as compared with the distance of interest  $r = |\mathbf{s}_2 - \mathbf{s}_1|$ .

## Appendix I. Matrix elements for hard walls

The position of a particle in the vicinity of a wall element can be described by  $Q = (z, \mathbf{s})$  where  $\mathbf{s}$  is a surface coordinate and  $z$  is a perpendicular ‘radial’ coordinate. The potential which is experience by the particle is assumed to be  $\mathcal{V}(Q) = 0$  inside the cavity where  $z < 0$ , and  $\mathcal{V}(Q) = f \cdot z$  for  $z > 0$  up to some maximal value  $\mathcal{V}_{\text{wall}}$  well inside the barrier. We assume  $E \ll \mathcal{V}_{\text{wall}}$  and therefore  $\mathcal{V}_{\text{wall}}$  should have no significance. The limit  $f \rightarrow \infty$  corresponds to hard walls. For deformation field  $\hat{\mathbf{V}}(\mathbf{s})$ , defined such that  $\hat{\mathbf{V}}\delta x$  is the displacement of a wall element, one obtains

$$\frac{\partial \mathcal{H}}{\partial x} = -(\mathbf{n}(\mathbf{s}) \cdot \hat{\mathbf{V}}(\mathbf{s})) \mathcal{V}_{\text{wall}} \delta(z) \quad (\text{I.1})$$

The orientation of each wall element is represented by the unit vector  $\mathbf{n}(\mathbf{s})$ . The logarithmic derivative of the wavefunction along the boundary is  $\varphi(\mathbf{s})/\psi(\mathbf{s})$  where  $\varphi(\mathbf{s}) = \mathbf{n} \cdot \nabla \psi$ . For  $z > 0$  the wavefunction  $\psi(Q)$  is a decaying exponential. Hence the logarithmic derivative of the wavefunction on the boundary should be equal to  $-\sqrt{2m\mathcal{V}_{\text{wall}}}/\hbar$ . Consequently one obtains the following expression for the matrix elements that are associated with the deformation:

$$\left( \frac{\partial \mathcal{H}}{\partial x} \right)_{nm} = -\frac{\hbar^2}{2m} \oint \varphi_n(\mathbf{s}) \varphi_m(\mathbf{s}) (\mathbf{n} \cdot \hat{\mathbf{V}}) ds \quad (\text{I.2})$$

For uncorrelated chaotic eigenstates we get by squaring (I.2) and using (H.3), the following expression:

$$\begin{aligned} \left\langle \left| \left( \frac{\partial \mathcal{H}}{\partial x} \right)_{nm} \right|^2 \right\rangle &= \left( \frac{1}{\text{Volume}} \right)^2 \times \left( \frac{(\hbar k)^2}{m} \right)^2 \times \\ &\times \oint \oint \text{Sinc}(k_n|\mathbf{s}_2 - \mathbf{s}_1|) \text{Sinc}(k_m|\mathbf{s}_2 - \mathbf{s}_1|) (\mathbf{n} \cdot \hat{\mathbf{V}}(\mathbf{s}_1)) ds_1 (\mathbf{n} \cdot \hat{\mathbf{V}}(\mathbf{s}_2)) ds_2 \end{aligned}$$

If De-Broglie wavelength is a small scale, then the difference  $|k_n - k_m|$  will have no significance in the calculation. Soft walls are essential in order to have finite bandwidth

(see next appendix). A classical look-alike result for  $\nu_E = \tilde{C}_E(0)$  is obtained by setting  $k_n \sim k_m \sim k$  and then multiplying by  $2\pi\hbar/\Delta$ . Assuming that  $\lambda_E$  is a small scale, it is possible to approximate the  $(\text{Sinc})^2$  by a delta function (see (D.7)) and consequently the semiclassical estimate that follows from (28) for individual matrix elements is recovered:

$$\left| \left( \frac{\partial \mathcal{H}}{\partial x} \right)_{nm} \right| \approx \frac{1}{\text{Volume}} \frac{(\hbar k)^2}{m} \sqrt{\frac{2\langle |\cos(\theta)|^3 \rangle}{\Omega_d}} \text{Area } \lambda_E^{d-1} \quad (\text{I.3})$$

Compared with non-chaotic eigenstate, for which  $\text{Sinc} \mapsto 1$ , there is a factor  $1/\sqrt{\mathcal{N}}$ , where  $\mathcal{N} = (\text{Area}/\lambda_E^{d-1})$  is the number of correlated regions on the surface of the cavity.

### Appendix J. Finite bandwidth due to soft walls

Equation (I.3) is valid for hard walls. For soft walls  $|(\partial \mathcal{H}/\partial x)_{nm}|^2$  should be multiplied by a suppression factor  $c_{\text{soft}} \leq 1$ . This suppression factor can be estimated by considering a plane wave incident upon the wall [5]. The result is

$$c_{\text{soft}} = \left| \frac{1}{\varepsilon_n - \varepsilon_m} \left( \frac{\sin \phi_n \cos \phi_m}{\sqrt{\varepsilon_n}} - \frac{\sin \phi_m \cos \phi_n}{\sqrt{\varepsilon_m}} \right) \right|^2 \quad (\text{J.1})$$

where  $\varepsilon = (k/(2mf/\hbar^2)^{1/3})^2$  is the scaled energy of the eigenstate. The reflection phase-shift is obtained via  $\tan(\phi) = (\mathcal{A}/\mathcal{A}')\sqrt{\varepsilon}$ . We define  $\mathcal{A} = \text{Airy}(-\varepsilon)$ , and  $\mathcal{A}'$  and  $\mathcal{A}''$  are the respective first and second derivatives. If  $\phi_n$  is very close to  $\phi_m$  then we can make the approximation

$$c_{\text{soft}} \approx \left[ \frac{(\mathcal{A}')^2 - (\mathcal{A}\mathcal{A}'')}{(\mathcal{A}')^2 + \varepsilon(\mathcal{A})^2} \right]^2 \quad (\text{J.2})$$

In the hard wall limit  $\varepsilon \rightarrow 0$ , and  $\mathcal{A}'' \rightarrow 0$ , consequently this factor will be equal unity as expected. If  $\varepsilon_n$  and  $\varepsilon_m$  are not very close, then  $\phi_n$  and  $\phi_m$  can be treated as uncorrelated and we obtain

$$c_{\text{soft}} \approx \frac{1}{2\varepsilon} \frac{1}{(\varepsilon_n - \varepsilon_m)^2} = 2 \left( \frac{\hbar}{\tau_{\text{cl}}} \right)^2 \frac{1}{(E_n - E_m)^2} \quad (\text{J.3})$$

The bandwidth can be estimated by finding the difference  $E_n - E_m$  for which the last expression becomes of order unity. This gives the result  $\Delta_b = \hbar/\tau_{\text{cl}}$  where  $\tau_{\text{cl}}$  is the collision time with the wall. This is in agreement with our semiclassical expectations. We learn that outside the band, the matrix element have a power-law decay. This result looks of semiclassical nature since it adds an  $\hbar$  independent factor to  $C_E(\omega)$ . A  $1/\omega^2$  tail of  $C_E(\omega)$  should be associated with a discontinuity of the first derivative of  $C_E(\tau)$  at  $\tau = 0$ . See App.Appendix E.

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