Fermi's Golden Rule and Exponential Decay as a RG Fixed Point

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Abstract We discuss the decay of unstable states into a quasicontinuum using Hamiltonian models. We show that exponential decay and the golden rule are exact in a suitable scaling limit, and that there is an associated renormalization group (RG) with these properties as a fixed point. The method is inspired by a limit theorem for infinitely divisible distributions in probability theory, where there is a RG with a Cauchy distribution, i.e. a Lorentz line shape, as a fixed point. Our method of solving for the spectrum is well known; it does not involve a perturbation expansion in the interaction, and needs no assumption of a weak interaction. Using random matrices for the interaction we show that the ensemble fluctuations vanish in the scaling limit. For non-random models we can use uniformity assumptions on the density of states and the interaction matrix elements to estimate the deviations from the decay rate defined by the golden rule.

Keywords Fermi's golden rule \cdot Renormalization group \cdot Feshbach method \cdot Random matrix \cdot Unstable states \cdot Lorentz line shape

1 Introduction

Fermi's golden rule gives a very successful recipe for calculating the decay rate of metastable quantum states. It often works much better than we could expect from the standard textbook treatment. One goal of this paper is to explain this surprising generality.

A general Hamiltonian describing the decay of a single quantum state $|\psi_s\rangle$ into a quasicontinuum of background states can be represented in the form

$$H = \begin{bmatrix} E_s & V \\ V^{\dagger} & H_B \end{bmatrix}$$
(1)

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where H_B is a Hermitian matrix, V is a row vector of interaction matrix elements, and $E_s = \langle \psi_s | H | \psi_s \rangle$ is the unperturbed energy of the unstable state. Our problem is then to find sufficient conditions on H_B and V to give exponential decay as a good approximation, that is

$$p(t) := \left| \langle \psi_s | e^{-iHt} | \psi_s \rangle \right|^2 \approx p(0) e^{-\Gamma t}$$
⁽²⁾

with a Fermi golden rule form for the decay rate

$$\Gamma = 2\pi\rho v^2 \tag{3}$$

Here v represents the (average) transition matrix element of V and ρ is the density of states (DOS) of H_B . The convention $\hbar = 1$ is used throughout. We also want to find a limit in which the exponential decay is exact.

The standard derivation of (3) starts from a perturbation expansion of the unitary evolution, keeping the lowest nontrivial order, and then sums over a dense set of final states. The formula is essentially contained in Dirac [8], see also [23]. The corresponding quantum amplitude $\langle \psi_s | e^{-iHt} | \psi_s \rangle$ is a Fourier transform of a Lorentz (Breit-Wigner) line shape function

$$f_C(x-a,\Gamma) := \frac{\Gamma}{2\pi} \frac{1}{(x-a)^2 + \Gamma^2/4}$$
(4)

We will show that there is a simple and general solution to the problem which does not depend on a perturbation expansion. This has been known for a long time for special models, but it is our goal give a demonstration which remains valid under quite general and physically relevant conditions. It needs only a few uniformity conditions on the spectrum of H_B and the matrix elements of V. Here a key element in understanding the universality of the golden rule and the exponential decay is the idea that the Lorentz line shape function (4) is a fixed point under a renormalization group (RG) of transformations on the family of Hamiltonians of the form (1).

The present approach was inspired by an important theorem of probability theory. There (4) is a Cauchy probability density (PD), an infinitely divisible stable distribution. It is the distribution of a properly scaled limit of an infinite sum of independent identically distributed random variables, see e.g. Feller's book [11]. For any initial distribution the limit depends only on two real parameters, (Γ , a) in (4). This is similar to the role of the normal distributions in the central limit theorem, but the limit is adapted to PDs with long tails.

A physicist would call the Cauchy PD a fixed point for a renormalization group (RG) of transformations on the space of PDs, see Sects. 2 and 3. Our thesis is that this is also a good way to approach the quantum problem; for this purpose we have to define a suitable set of scaling transformations for the RG.

Many attempts at a rigorous derivation of rate equations (and quantum Markov master equations) use the van Hove limit, where there is a scaling of the interaction matrix elements (v) and the time (t) as follows

$$v \to \lambda v, \qquad t \to \lambda^{-2} t$$
 (5)

where $\lambda \to 0$ [5, 6, 21, 22]. In this way the dimensionless quantity Γt is invariant, but after the scaling the decay is on the rescaled (slow) time. Before taking such a limit it is necessary to let the DOS ρ be infinite, otherwise there would be no relaxation in the limit $\lambda \to 0$. Here we will instead use the scaling

$$v \to \lambda v, \qquad \rho \to \lambda^{-2} \rho$$
 (6)

where $\lambda \to 0$, Γ is invariant, and *t* does not scale. The name continuum, or statistical, limit is often used, but note that here all eigenstates are normalized and the spectrum is always discrete (a quasicontinuum). The dimensionless number

$$N_{\Gamma} := \rho \Gamma \tag{7}$$

scales as $N_{\Gamma} \rightarrow \lambda^{-2} N_{\Gamma}$, and has a natural interpretation as the number of states under the resonance width. It is also the number of matrix elements effectively involved in the transition, a natural large parameter for the limit (6). We could replace the small parameter λ by $N_{\Gamma}^{-1/2}$.

We will show that (6) is the relevant scaling both for the limit theorem for the Cauchy PD, and for the quantum models introduced in Sect. 4, and that the scaling can be interpreted as the iteration of a RG. In the scaling limit $\lambda = 0$ the DOS is clearly ∞ , and this is necessary in order to have exponential relaxation for long time scales. On the other hand, in order to have exponential relaxation for short time scales, it is necessary to have an unbounded energy spectrum for the Hamiltonian. We will perform the limit of an unbounded spectrum after the scaling (6), an order which appears most relevant for physical applications. This results in exponential relaxation, with a rate given by the golden rule (3) or a matrix generalization of this formula. Solving models of the type (1) directly for an unbounded continuous spectrum would meet with great mathematical difficulties, without being more physically relevant.

An outline of the contents is as follows.

We first sketch the properties of the Cauchy PD in Sects. 2 and 3. In Sect. 4 we give some known properties of models of the type (1). The spectral density for the relaxation is found, without any kind of expansion or approximation, using what is often known as the Feshbach method [12, 13]. The models are defined as an ensemble of random matrices; in the simplest case the ensemble is defined by just two variable (non-random) parameters ρ and v.

The case of a single level decaying into a quasicontinuum, is covered in Sect. 5. For the mathematical reasons mentioned above we perform the calculations for the case where the unperturbed spectrum lies in an energy interval Δ with a finite energy range ΔE . We calculate the ensemble averages of the functions representing the linewidth and the level shift and show that they have the desired properties in the scaling limit (7).

In Sect. 6 the variance of the fluctuations around the ensemble averages are estimated and shown to converge to zero in the scaling limit. When we let $\Delta \rightarrow \mathbb{R}$ the scaling limit of the spectral density is a Lorentzian with relaxation rate Γ defined by (3). We also get a measure of how good this is as an approximation for finite parameter values; a result that enhances the physical relevance of the models. In particular, if $N_{\Gamma} \gg 1$ and $\Gamma \ll \Delta E$, the exponential relaxation is still a good approximation. The calculations also show that the statistical ensembles can be dispensed with and replaced by uniformity assumptions on the spectra and interaction matrix elements. This allows us to examine a single Hamiltonian and estimate the suitability of using the golden rule, based only on averages calculated over a finite matrix.

In Sect. 7 the relation between the scaling (6) and the RG for the matrix models is analyzed. In Sect. 8 the unitary invariance of the random matrix ensemble is used to show that the results will hold for more general forms of the interaction. This invariance also allows us to show how the properties of the Cauchy distribution under convolution are related to those of the spectral density. In Sect. 9 we sketch how the models can describe several decaying states. There the Lorentz line shape need not apply, but there is a close relation to Fano's theory of lineshape. Section 10 spells out the limits to exponential decay posed by a finite spectral range or a discrete spectrum. Finally there are some conclusions and additional remarks in Sect. 11.

2 Properties of the Cauchy Distribution

The Lorentz line shape functions (4) form a family of Cauchy PDs on \mathbb{R} , with parameters $a \in \mathbb{R}$ and $\Gamma > 0$ and normalization

$$\int_{\mathbb{R}} dx f_C(x, \Gamma) = 1$$

Note that the mean and variance are not defined! The distribution function for a = 0 is

$$F_C(y,\Gamma) = \int_{-\infty}^{y} dx f_C(x,\Gamma) = \frac{1}{2} + \frac{1}{\pi} \arctan\left[\frac{2y}{\Gamma}\right]$$
(8)

When $\Gamma \to 0$ the limit is a unit step function, $F_C = 0$ for y < 0, and $F_C = 1$ for y > 0. Of course $F_C(-\infty, \Gamma) = 0$ and $F_C(\infty, \Gamma) = 1$ for all $\Gamma \ge 0$. The functions (4) form a convolution semigroup

$$\int_{\mathbb{R}} dx f_C(x - a_1, \Gamma_1) f_C(y - a_2 - x, \Gamma_2) = f_C(y - a_1 - a_2, \Gamma_1 + \Gamma_2)$$
(9)

see [11] Sect. 2.4. Thus, if two independent RVs X_1 and X_2 have Cauchy PDs with parameters Γ_1 and Γ_2 , then $X_1 + X_2$ has a Cauchy PD with parameter $\Gamma_1 + \Gamma_2$. For N independent RVs $\{X_1, X_2, \ldots, X_N\}$, all with the same Cauchy PD with parameter Γ , the sum is Cauchy with parameter N Γ and the average is Cauchy with parameter Γ

$$\frac{1}{N}S_N = \frac{1}{N}\sum_{k=1}^N X_k \sim X_1$$
(10)

where \sim indicates equality in distribution. The characteristic function is

$$\chi(t) := \int_{\mathbb{R}} dx f_C(x - a, \Gamma) \exp(-ixt) = \exp\left[-iat - \frac{1}{2}\Gamma|t|\right]$$
(11)

The convolution (9) corresponds to a multiplication of the characteristic functions.

Let the RVs in (10) have a common distribution F. Even when F is not Cauchy the scaled sum (10) can converge to a limit

$$X_{\infty} := \lim_{N \to \infty} \frac{1}{N} S_N \tag{12}$$

with a Cauchy distribution. Sufficient conditions on F for convergence can be found in [11] Sect. 17.5, especially in the Concluding remark, involving an assumption on the "tails" of F. The simplest case is that the following two limits exist and are equal

$$\lim_{x \to \infty} x \left[1 - F(x) \right] = \lim_{x \to \infty} x F(-x) = \frac{\Gamma}{2\pi}$$
(13)

where we can already identify the Cauchy parameter Γ . We let χ_F denote the characteristic function of *F* and define a sequence of centering constants (with a dimensional parameter γ)

$$\beta_k := \gamma \int_{\mathbb{R}} \sin(x/k\gamma) F(dx), \quad k \in \mathbb{Z}_+$$
(14)

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It follows from (13) that the following limit exists [11]

$$\lim_{n \to \infty} \left[\chi_F(t/n) \mathrm{e}^{i\beta_n t} \right]^n = \mathrm{e}^{-|t|\Gamma/2} \tag{15}$$

The statement for the distribution F corresponding to (15) is

$$F_{\infty}(x) := \lim_{n \to \infty} (*^{n} F)[n(x + \beta_{n})] = F_{C}(x, \Gamma)$$
(16)

We note the similarity to the central limit theorem, but there the factor 1/N in (12) is replaced by $1/\sqrt{N}$. If *F* has zero mean and a finite second moment then there is a convergence to a normal distribution, see [11], Sect. 8.4. A RG version of the central limit theorem is described in [17]. On the other hand for an *F* with a finite second moment the limit (16) is a step function corresponding to a δ -function density.

3 An Example

We now want to give an intuitive hint why the mathematical result in the previous section is connected to the quantum lineshape problem. As an example of a distribution which fulfills (13) we pick one which is obtained from a standard lowest order perturbation expansion. Consider an infinite set of unperturbed quantum states $\{|k\rangle, k \in \mathbb{Z}\}$, with energy eigenvalues $E_k = k\omega$. There is a perturbation V with nonzero matrix elements $\langle 0|V|k\rangle = v, \forall k \neq 0$. The perturbed state $|\psi_0\rangle$ which converges to $|0\rangle$ as $v \to 0$ has the occupation numbers, to the order v^2

$$p_k := |\langle k | \psi_0 \rangle|^2 = \frac{v^2}{k^2 \omega^2} \quad (k \neq 0), \qquad p_0 := 1 - 2\sum_{k=1}^{\infty} p_k \tag{17}$$

where v^2 must be small enough to make $p_0 > 0$, i.e. $v^2 \le 3\pi^{-2}\omega^2$. The distribution is a step function with steps at $x = k\omega$

$$F(x) = \sum_{k\omega < x} p_k$$

and centered, hence (14) is zero. We find that the first limit in (13) reads

$$\frac{v^2}{\omega^2}\lim_{x\to\infty} x\sum_{k\omega\ge x}\frac{1}{k^2} = \frac{v^2}{\omega^2}\lim_{x\to\infty} x\int_{y\omega\ge x}\frac{dy}{y^2} = \frac{v^2}{\omega} = \rho v^2 = \frac{\Gamma}{2\pi}$$

and the second limit is identical; consequently we know that (16) holds with $\beta_n = 0$.

Note that F * F has steps separated by ω , while (F * F)[2x] has steps separated by $\omega/2$, and $(*^n F)(nx)$ in (16) has steps separated by ω/n . On the other hand we know from (9) if Fis Cauchy then this convolution and rescaling recovers F. Consequently, this is an example of the scaling (6), when we identify Γ with (3).

As a preparation for later developments we consider a generalization to random distributions. Let V have random matrix elements $\langle 0|V|k \rangle = \xi_k$ where the RVs ξ_j are assumed to be complex-valued, normal, and independent, defined by the first two moments

$$\langle \xi_k \rangle = 0, \qquad \left\langle \xi_j^* \xi_k \right\rangle = v^2 \delta_{jk} \tag{18}$$

The distribution function is now itself a random function. Consider the distribution of the tail function

$$T(x) := 1 - F(x) = \frac{1}{\omega^2} \sum_{k\omega \ge x} \frac{|\xi_k|^2}{k^2}$$

Clearly the ensemble average gives back what we had before

$$\lim_{x \to \infty} x \left\langle T(x) \right\rangle = \frac{\Gamma}{2\pi}$$

We can also calculate the ensemble variance. Introduce the real random vector

$$\eta_k := |\xi_k|^2 - v^2 \tag{19}$$

and use the standard properties of the normal RVs ξ to calculate

$$\langle \eta_k \rangle = 0, \qquad \langle \eta_j \eta_k \rangle = \delta_{jk} v^4$$
(20)

Define

$$\Delta T(x) := T(x) - \langle T(x) \rangle = \frac{1}{\omega^2} \sum_{k\omega \ge x} \frac{\eta_k}{k^2}$$

Then $\langle \Delta T(x) \rangle = 0$ and for large x the leading term of the variance is

$$\langle \Delta T(x)^2 \rangle = \frac{1}{\omega^4} \sum_{k\omega \ge x} \frac{v^4}{k^4} \approx \frac{v^4}{\omega^4} \int_{y\omega \ge x} \frac{dy}{y^4} = \frac{v^4}{3\omega x^3}$$

and it follows that

$$\lim_{x \to \infty} x^2 \langle \Delta T(x)^2 \rangle = \lim_{x \to \infty} \frac{v^4}{3\omega x} = 0$$

Using Chebyshev's inequality ([11], Chap. 5) we find for every $0 < \alpha < 1/2$, $\delta > 0$

$$\operatorname{Prob}\left\{|x\Delta T(x)| \ge x^{-\alpha}\delta\right\} \le x^{2(1+\alpha)}\delta^{-2}\left(\Delta T(x)^{2}\right) \approx \frac{1}{3}\frac{v^{4}}{\delta^{2}\omega}x^{2\alpha-1}$$

and this expression goes to zero as $x \to \infty$. The same argument applies to the limit $x \to -\infty$. From these estimates it can be concluded that (13), (15) and (16) will hold in probability. However, the centering constants (14) can not be left out.

4 Matrix Models and Resolvents

In this section we review some properties of Hamiltonians like (1) or the block matrix generalization

$$H = \begin{bmatrix} H_A & V \\ V^{\dagger} & H_B \end{bmatrix}$$
(21)

These facts are known, the main ideas going back at least to Feshbach [12, 13, 18]. The mathematical background can be traced from Remark 2.1 of [16]. There are also textbook treatments with physical applications, see [3], Complements C_I and C_{III} , and [20], Chap. 21. However, later on we will use the results in a way which seems not to be standard.

For now we assume the Hilbert space to be of finite dimension, and the eigenstates are all normalized. In the limit $\lambda \rightarrow 0$ in (6) the dimension is infinite, and the same holds when the energy spectrum is unbounded. These limits will be discussed later.

Let the Hamiltonian *H* have a discrete spectrum $\{\omega_{\nu}\}$, assumed non-degenerate for simplicity, and spectral projectors $\{P_{\nu}\}$

$$H:=\sum_{\nu}\omega_{\nu}P_{\nu}$$

Define a causal resolvent (Green's function) with a regularization parameter $\varepsilon > 0$

$$R(z-i\varepsilon) := (z-i\varepsilon - H)^{-1} = \sum_{\nu} (z-i\varepsilon - \omega_{\nu})^{-1} P_{\nu}$$

We can pick a number of the projectors by integrating over a counterclockwise contour encircling the poles with real parts in a finite interval $I \subset \mathbb{R}$: $\{z = \omega_{\nu} + i\varepsilon, \omega_{\nu} \in I\}$

$$\sum_{\omega_{\nu}\in I} P_{\nu} = \frac{1}{2\pi i} \oint dz \ R(z - i\varepsilon)$$

For small ε we can approximate the contour integral by one along the real axis

$$\frac{1}{2\pi i} \int_{I} dx [R(x - i\varepsilon) - R(x + i\varepsilon)] = \frac{1}{\pi} \int_{I} dx \operatorname{Im} R(x - i\varepsilon)$$

This means that we can consider the function

$$\frac{1}{\pi} \operatorname{Im} R(x - i\varepsilon) = \frac{1}{\pi} \sum_{\nu} \frac{\varepsilon}{(x - \omega_{\nu})^2 + \varepsilon^2} P_{\nu}$$
(22)

as a regularized spectral density, normalized as follows

$$\frac{1}{\pi} \int_{\mathbb{R}} dx \operatorname{Im} R(x - i\varepsilon) = \sum_{\nu} P_{\nu} = \mathbb{1}$$

and the trace of (22) is a regularized DOS. The regularization can be written as a convolution (averaging) by a Cauchy PD

$$\operatorname{Im} R(x - i\varepsilon) = \lim_{\delta \to 0} \int_{\mathbb{R}} dy f_C(x - y, \varepsilon) \operatorname{Im} R(y - i\delta)$$

The regularization can be justified by noting that the duration of an observation of the system is bounded by a time scale $1/\varepsilon$, assumed much longer than the decay time.

Now use the form (21) and introduce the projectors Π_A , $\Pi_B = \mathbb{1} - \Pi_A$ on the complementary subspaces. We know from the properties of the Schur complement [4] that

$$R_A(x-i\varepsilon) := \prod_A R(x-i\varepsilon) \prod_A = [x-i\varepsilon - \hat{H}_A(x-i\varepsilon)]^{-1}$$
(23)

where, for any $z \in \mathbb{C}$, we define a non-Hermitian effective Hamiltonian

$$\tilde{H}_{A}(z) := H_{A} + V(z - H_{B})^{-1} V^{\dagger} = \tilde{H}_{A}(z^{*})^{\dagger}$$
(24)

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We find for the imaginary part of (23), which, with a factor $1/\pi$, is the spectral density (22) projected on the subspace A

$$\phi_A(x,\varepsilon) := \frac{1}{\pi} \operatorname{Im} R_A(x-i\varepsilon)$$
$$= \frac{1}{\pi} R_A(x-i\varepsilon) \Big[\varepsilon + \operatorname{Im} \tilde{H}_A(x-i\varepsilon) \Big] R_A(x-i\varepsilon)^{\dagger}$$
(25)

For all $\varepsilon > 0$, $x \in \mathbb{R}$ this is a positive definite matrix. The Fourier transform is the matrixvalued characteristic function

$$\chi_A(t,\varepsilon) := \int_{\mathbb{R}} dx \exp(-ixt)\phi_A(x,\varepsilon)$$
(26)

We also define the distribution function

$$\Phi_A(x,\varepsilon) := \int_{-\infty}^x dy \phi_A(y,\varepsilon)$$
(27)

Note that the normalization implies that for every ε ,

$$\Phi_A(-\infty,\varepsilon) = 0, \qquad \Phi_A(\infty,\varepsilon) = \mathbb{1}_A$$

When $\varepsilon \to 0$ (27) converges to a step function $\Phi_A(x, 0)$; the steps are at $x = \omega_v$, the spectrum of H.

We can see in (25) the beginning of an exponential relaxation. In fact, if we could assume that $\tilde{H}_A(x - i\varepsilon)$ is independent of x, then (26) is a matrix-valued decaying amplitude

$$\chi_A(t,\varepsilon) = \exp\left(-it\operatorname{Re}\ddot{H}_A - |t|\varepsilon - |t|\operatorname{Im}\ddot{H}_A\right)$$
(28)

Our goal is to justify this simple form in the limit (6), where we can finally set $\varepsilon = 0$. In most of the calculations below we will let the subspace A have rank 1, and then, if we leave out the argument $x - i\varepsilon$, the projected spectral density simplifies to

$$\phi_A(x,\varepsilon) = \frac{1}{\pi} \frac{\varepsilon + \operatorname{Im} \tilde{H}_A(x-i\varepsilon)}{(x - \operatorname{Re} \tilde{H}_A(x-i\varepsilon))^2 + (\varepsilon + \operatorname{Im} \tilde{H}_A(x-i\varepsilon))^2}$$
(29)

Again, if $\tilde{H}_A(x - i\varepsilon)$ is constant we have the resonance form (4).

Note that the ε -averaged form of the resolvent (25) is expressed in terms of another ε -averaged quantity, Im $\tilde{H}_A(x - i\varepsilon)$. This fact simplifies the calculations and the interpretation of the calculated quantities.

5 The Basic Hamiltonian

In (21) let the subspace indexed A have rank 1, thus the Hamiltonian has the form (1). For special choices of V case has been solved repeatedly in the past and used for numerous applications, see for example [1, 3, 7, 10, 15]. We will let the interaction V represent a vector of independent random variables, a device often used in applications [2, 19]. Here it will allow us to make statements about the solutions valid in limits where the ensemble fluctuations vanish.

In the Hamiltonian (1) it is no restriction to assume H_B diagonal with elements E_j and spanned by a finite set of states { $|j\rangle$; $j = -N_B, -N_B + 1, ..., N_B$ }. First choose an equidistant spectrum $E_j = E_0 + j\omega_B$ where $E_0 \approx E_s$. The calculations will show that we can cope with more general spectra with an average DOS $\rho_B = 1/\omega_B$. We also assume that the energies are restricted to a finite interval Δ of width $\Delta E = E_+ - E_-$

$$E_j \in \Delta := [E_-, E_+]$$

Only a lower bound is essential for finite quantum systems, but here we prefer to simplify the mathematics by having a finite number of states in H_B , $N_B = 1 + \rho_B \Delta E$; later we can let this number approach ∞ .

We choose the components of V in (1) to be independent complex normal random variables

$$\langle \psi_s | V | j \rangle = \langle j | V | \psi_s \rangle^* = \xi_j \tag{30}$$

defined by (18), while all other matrix elements are zero. The spectral density (29) is now

$$\frac{1}{\pi} \langle \psi_s | \operatorname{Im} R(x - i\varepsilon) | \psi_s \rangle = \frac{\varepsilon}{\pi} \sum_{\nu} \frac{|\langle \psi_s | \omega_{\nu} \rangle|^2}{(x - \omega_{\nu})^2 + \varepsilon^2}$$
(31)

and in the limit $\varepsilon \to 0$ the Fourier transform (26) is the amplitude for staying in the state $|\psi_s\rangle$:

$$\langle \psi_s | \exp(-iHt) | \psi_s \rangle = \sum_{\nu} |\langle \psi_s | \omega_{\nu} \rangle|^2 \exp(-it\omega_{\nu})$$

For given E_s , H_B and V the equation system to solve for the eigenvalues ω_{ν} and eigenvectors $|\omega_{\nu}\rangle$ is [1]

$$(E_s - \omega)\langle \psi_s | \omega \rangle + \sum_j \xi_j \langle j | \omega \rangle = 0$$
$$(E_k - \omega)\langle k | \omega \rangle + \xi_k^* \langle \psi_s | \omega \rangle = 0$$

We know that each eigenvalue ω_{ν} is located between two unperturbed (V = 0) eigenvalues, but we do not need the exact values. Instead we can estimate the terms in the RHS of (29). Decompose (24) into real and imaginary parts, for insertion in (29).

$$\tilde{H}_A(x-i\varepsilon) = E_s + \sum_j \frac{|\xi_j|^2 (x-E_j)}{(x-E_j)^2 + \varepsilon^2} + i\varepsilon \sum_j \frac{|\xi_j|^2}{(x-E_j)^2 + \varepsilon^2}$$
(32)

We first deal with the imaginary part

$$\operatorname{Im} \tilde{H}_{A}(x - i\varepsilon) = \varepsilon \sum_{j} \frac{|\xi_{j}|^{2}}{(x - E_{j})^{2} + \varepsilon^{2}}$$
(33)

A simpler case is solved e.g. in [1], where the interaction is non-random, $\xi_j = v$, and the spectrum of H_B is unbounded, i.e. $E_{\pm} = \pm \infty$. When $\omega_B \ll \varepsilon$ the infinite sum is approximated by an integral which is independent of the argument in \tilde{H}_A

Im
$$\tilde{H}_A \approx \frac{\varepsilon v^2}{\omega_B} \int_{\mathbb{R}} dy \frac{1}{y^2 + \varepsilon^2} = \pi \rho_B v^2 = \frac{\Gamma}{2}$$
 (34)

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where we have put $\rho = \rho_B$ in (3). For our model, first apply the ensemble average over the RVs ξ_i , then, again, approximate by an integral

$$\left\langle \operatorname{Im} \tilde{H}_{A} \right\rangle = \varepsilon v^{2} \sum_{j} \frac{1}{(x - E_{j})^{2} + \varepsilon^{2}} \approx \frac{\Gamma}{2} J(x, \varepsilon)$$
$$J(x, \varepsilon) := \frac{\varepsilon}{\pi} \int_{E_{-}-x}^{E_{+}-x} dy \frac{1}{y^{2} + \varepsilon^{2}} = \arctan\left[\frac{E_{+}-x}{\varepsilon}\right] - \arctan\left[\frac{E_{-}-x}{\varepsilon}\right] \quad (35)$$

It is easiest to see the behavior of the function J by a computer calculation. For $\varepsilon \ll \Delta E$ it is close to the indicator function $\chi(\Delta, x)$ for the interval Δ , with deviations ε -near the end points. When $\varepsilon \to 0$ then $J(x, \varepsilon) \to \chi(\Delta, x)$ and

$$\left\langle \operatorname{Im} \tilde{H}_A(x-i\varepsilon) \right\rangle \approx J(x,\varepsilon) \frac{\Gamma}{2} \to \chi(\Delta,x) \frac{\Gamma}{2}$$
 (36)

The same method applies to the real part

$$\left\langle \operatorname{Re} \tilde{H}_{A} \right\rangle = E_{s} + v^{2} \sum_{j} \frac{(x - E_{j})}{(x - E_{j})^{2} + \varepsilon^{2}} \approx E_{s} + \Gamma K(x, \varepsilon)$$
$$K(x, \varepsilon) := \frac{1}{2\pi} \int_{E_{--x}}^{E_{+-x}} dy \frac{y}{y^{2} + \varepsilon^{2}} = \frac{1}{4\pi} \ln \left[\frac{(E_{+} - x)^{2} + \varepsilon^{2}}{(E_{-} - x)^{2} + \varepsilon^{2}} \right]$$
(37)

The second term in (37) represents an x-dependent level shift; it has a well-defined limit when $\varepsilon \to 0$. It has the effect of changing the DOS slightly, on the order of $\Gamma/\Delta E$. Near the center $\bar{x} = (E_+ + E_-)/2$ of Δ and for large ΔE

$$K(x,0) = \frac{1}{2\pi} \ln \left[\frac{\Delta E - 2(x - \bar{x})}{\Delta E + 2(x - \bar{x})} \right] \approx -\frac{2}{\pi} \frac{x - \bar{x}}{\Delta E}$$
(38)

There is no unique way of taking the limit $\Delta E \to \infty$, but as long as x and \bar{x} stay bounded, it holds for all fixed $\varepsilon \ge 0$ that

$$\lim_{\Delta E \to \infty} K(x, \varepsilon) = 0 \tag{39}$$

Summing up the results so far: if we use the ensemble averages derived above for the terms in (29), and replacing the sums with integrals, we find the following approximation which we expect to be good for $\omega_B \ll \varepsilon$ (cf. [3], Complement C_{III})

$$\phi_A(x,\varepsilon) \approx \frac{1}{2\pi} \frac{2\varepsilon + \Gamma J(x,\varepsilon)}{[x - E_s - \Gamma K(x,\varepsilon)]^2 + [2\varepsilon + \Gamma J(x,\varepsilon)]^2/4}$$
(40)

6 Estimating the Ensemble Fluctuations

We want to show that the fluctuations around the ensemble averages of the previous section and the error of replacing sums by integrals vanish in the limit (6). Thus, in this limit Im \tilde{H}_A and Re \tilde{H}_A are given by the last terms of (35) and (37), and the spectral density (40) is exact. We will concentrate on Im \tilde{H}_A , since the real part is very similar. The deviation from the ensemble mean is given by

$$\Delta \operatorname{Im} \tilde{H}_A := \operatorname{Im} \tilde{H}_A - \left\langle \operatorname{Im} \tilde{H}_A \right\rangle = \varepsilon \sum_j \frac{\eta_j}{(x - E_j)^2 + \varepsilon^2}$$

where η is the RV (19), with mean and variance given by (20). The variance of (33) is

$$\sigma^{2}\left(\operatorname{Im}\tilde{H}_{A}\right) := \left\langle \left(\Delta\operatorname{Im}\tilde{H}_{A}\right)^{2} \right\rangle = \varepsilon^{2}v^{4}\sum_{j}\left[(x-E_{j})^{2}+\varepsilon^{2}\right]^{-2}$$

For an order of magnitude estimate we again replace the sum by an integral, and extend the integral to \mathbb{R} . Calculations similar to those performed above give

$$\sigma^2 \left(\operatorname{Im} \tilde{H}_A \right) \approx \frac{\pi v^4}{2\varepsilon \omega_B} = \frac{\omega_B}{2\varepsilon} \frac{\Gamma^2}{4\pi}$$
(41)

For the relative size of the fluctuations we can take the square root of this expression over (34), estimating the importance of the correction due to these fluctuations by the dimensionless parameter

$$\kappa := \sqrt{\frac{\omega_B}{2\pi\varepsilon}} = \frac{1}{\sqrt{2\pi N_\varepsilon}} \tag{42}$$

where $N_{\varepsilon} := \rho_B \varepsilon$. From (6) follows that it scales as $\kappa \to \lambda \kappa$ and goes to zero. Similar calculations show that κ also measures the fluctuations in Re \tilde{H}_A . We again use the Chebyshev inequality for an upper bound on the probability of having a deviation from the ensemble average [11]

Probability{
$$|\Delta \operatorname{Im} \tilde{H}_A| \ge \delta$$
} $\le \frac{1}{2\pi N_{\varepsilon}} \left[\frac{\Gamma}{2\delta}\right]^2$

Clearly, this quantity scales as λ^2 , and the (7) will give a value for Im \tilde{H}_A and Re \tilde{H}_A equal to the ensemble average.

We also have to estimate the error involved in replacing the sum over the spectrum by an integral, and in the assumptions on the level spacing. If the statistics for the level spacings form a Poisson process with parameter ρ_B , then the expected number of levels in an interval δE and the variance are equal

$$\langle N_{\delta E} \rangle = \rho_B \delta E = \sigma^2(N) := \langle (N_{\delta E} - \rho_B \delta E)^2 \rangle$$

Using the random version of the sequence $\{E_j\}$ in a sum like (32), we get the relative size of the resulting fluctuations by setting $\delta E = \varepsilon$

$$\frac{\sigma^2(N)}{\langle N \rangle^2} = \frac{1}{\rho_B \varepsilon} = \frac{\omega_B}{\varepsilon}$$
(43)

The square root is of the same order as κ (42). If we use a uniformly spaced spectrum the integral approximation has a smaller error, of order (43) squared. We know that random matrix spectra are typically more uniform than the Poisson case; this is the feature of "spectral rigidity" due to level repulsion [19]. The correction term will then be in between the uniform and Poisson values. The Poisson value can be considered a worst case for ensembles of





spectra with a given ensemble average DOS. The argument so far justifies (40) as an exact result in the limit (6).

What happens when the limits $\varepsilon \to 0$ and $\Delta \to \mathbb{R}$ are taken after (6)? The order of taking these two limits is not essential here. The limit $\varepsilon \to 0$ is straightforward in (40), and we get a normalized density $\phi_A(x, 0)$. This is a modified Cauchy density in a finite spectral interval and with a level shift function from (37) and (38). Finally, in the limit $\Delta \to \mathbb{R}$, using (39), we recover the exact Cauchy form

$$\lim_{\Lambda \to \mathbb{R}} \phi_A(x,0) = f_C(x - E_s, \Gamma) \tag{44}$$

In view of the fact that many applications involve models with large but finite DOS ρ_B , it is also interesting to see what we can say in this case, when we let $\varepsilon \to 0$ while $N_{\Gamma} \gg 1$. It is then convenient to use the integrated distribution function (27), which is always finite and monotonically increasing, while ϕ_A is a sum of δ -functions. Thus $\Phi_A(x, 0)$ is a step function, while the ε -averaged version $\Phi_A(x, \varepsilon)$ is close, as measured by the small number (42), to a Cauchy distribution (8) for $1 \ll N_{\varepsilon} \ll N_{\Gamma}$ and $\Gamma \ll \Delta E$. Given the properties of the two spectral densities, the local averaging on an energy scale ε cannot have a drastic effect, and it must hold that

$$\Phi_A(x,0) \approx F_C(x - E_s, \Gamma) \tag{45}$$

is a good approximation. This statement is supported by numerical calculations, see Fig. 1. We can conclude that the distribution calculated from the model is close to Cauchy if there is a clear separation of energy scales

$$\omega_B \ll \Gamma \ll \Delta E \tag{46}$$

which also implies that $N_{\Gamma} \gg 1$.

To reach these conclusions, the properties of the spectrum of H_B and of the matrix elements of V were crucial. So far we have assumed simple regular or random distributions to do our estimates. Similar calculations are possible for more general sequences $\{E_j\}$ and $\{\xi_k\}$ without an assumed statistical distribution. Instead we can postulate a uniformity for the spectrum and the matrix elements, a property which could in principle be verified in a

concrete model. For the level spacing assume that the following estimate holds uniformly in *x*, for all $\varepsilon \gg \omega_B$ and with κ defined by (42),

$$\frac{\omega_B \varepsilon}{\pi} \sum_j \frac{1}{(x - E_j)^2 + \varepsilon^2} = 1 + O(\kappa)$$
(47)

When $\varepsilon \to \infty$ (or $\varepsilon \to \Delta E$) the RHS must be essentially unity, and this fixes ω_B . In the same way the uniformity of the matrix elements means that

$$\frac{\omega_B \varepsilon}{\pi v^2} \sum_j \frac{|\xi_j|^2}{(x - E_j)^2 + \varepsilon^2} = 1 + O(\kappa)$$
(48)

where v^2 is defined through the limit $\varepsilon \to \infty$. The factor before the sum is $2\varepsilon/\Gamma$.

7 Scaling and Renormalization

It is now easy to see how the scaling (6) works in the models of the type (21). If we disregard mathematical rigor the simplest form is obtained when the energy interval $\Delta = \mathbb{R}$. Then *H* in (21) transforms in a simple way: for $0 < \lambda < 1$

$$\begin{bmatrix} H_A & V \\ V^{\dagger} & H_B \end{bmatrix} \longrightarrow \begin{bmatrix} H_A & \lambda V \\ \lambda V^{\dagger} & \lambda^2 H_B \end{bmatrix}$$
(49)

Clearly these transformations form a semigroup, and we think of them as a RG. We can let H_B and V be random or not; it is enough that they fulfill the uniformity properties (47) and (48), which are preserved under the transformations. Of course, there is no proper limit for (49) as $\lambda \rightarrow 0$. For any initial choice of H of the type indicated above there a limit for Φ_A of the Cauchy form, and this is then the "fixed point" of the RG (49).

When $\Delta = \mathbb{R}$ we can also explore the relation of the RG transformation (49) with that defining the Cauchy PD limit in Sect. 3. For large *x* the tail function of (27) is

$$T(x,\varepsilon) := 1 - \Phi_A(x,\varepsilon) \approx \frac{1}{\pi} \int_x^\infty dy \ y^{-2} \left[\varepsilon + \operatorname{Im} \tilde{H}_A(y-i\varepsilon) \right]$$

For simplicity, again assume that the spectrum of H_B is $\{k\omega_B, k \in \mathbb{Z}\}$. Then a straightforward calculation gives

$$\lim_{\varepsilon \to 0} T(x,\varepsilon) = \frac{1}{\omega_B^2} \sum_{k \omega_B \ge x} \frac{|\xi_k|^2}{k^2}$$

Comparing with the calculations in Sect. 3 we again find the tail condition (13) with strong convergence

$$\lim_{x \to \infty} xT(x,0) = \frac{\Gamma}{2\pi}$$

Hence, setting $\Phi_A(x, 0) = F(x)$ we find that (15) and (16) hold. The two limiting procedures, that applied to the quantum models and that applied to PDs, give the same limits for an infinite uniform spectrum. The same result holds for a spectrum that is a stationary Poisson process.

We would like to define a RG transformation when Δ is a finite interval. For this purpose we choose a scaling (6) with $\lambda = 1/\sqrt{2}$, this clearly involves a doubling of the dimension of the matrices. Explicitly, consider a matrix (21) composed of three parts, where the assumptions on H_A and the other components are as in Sect. 5

$$H = \begin{bmatrix} H_A & V_B & V_C \\ V_B^{\dagger} & H_B & 0 \\ V_C^{\dagger} & 0 & H_C \end{bmatrix}$$
(50)

We note the matrix identity

$$\begin{bmatrix} V_B, V_C \end{bmatrix} \begin{bmatrix} H_B & 0 \\ 0 & H_C \end{bmatrix}^{-1} \begin{bmatrix} V_B, V_C \end{bmatrix}^{\dagger} = V_B H_B^{-1} V_B^{\dagger} + V_C H_C^{-1} V_C^{\dagger}$$

and the corresponding decomposition of the effective Hamiltonian

$$\tilde{H}_A(z) = H_A + V_B(z - H_B)^{-1} V_B^{\dagger} + V_C(z - H_C)^{-1} V_C^{\dagger}$$

Thus the contributions of *B* and *C* to Im \tilde{H}_A and to the decay of *A* just add up. Clearly $\rho_{B+C} = \rho_B + \rho_C$. We can assume Poisson statistics for H_B and H_C with parameters ρ_B and ρ_C . For B + C the statistics will then be Poisson with parameter ρ_{B+C} . Let the transformation be represented by

$$H_B \to H_{B+B'}, \qquad V \to \frac{1}{\sqrt{2}} \left[V, V' \right]$$
 (51)

where H_B and $H_{B'}$ have the same DOS ρ_B and independent Poisson statistics, while V and V' both have the distribution defined in (18). The number of energy levels scales as $N \rightarrow 2N$. The RG is an iteration of the dimension doubling, hence a sequence $\lambda_k = 2^{-k/2}\lambda_0 \rightarrow 0$, obtaining the limit discussed in Sect. 6, when we set $\varepsilon = 0$.

8 Scaling and Convolution

In this section we will indicate the relation between the convolution property (9) of the Cauchy distribution and the scaling properties of another family of quantum models. The non-rigorous argument is based on the results of the previous sections and is supported by numerical simulations. Consider Hamiltonians of the form

$$H_1 = H_0 + V \tag{52}$$

where H_0 is a diagonal matrix with properties like those of H_B in (21). Again let E_k and $|k\rangle$ be the eigenvalues and eigenvectors of H_B , while the DOS is ρ_0 , and the spectral interval Δ . The eigenvalues and eigenvectors of H_1 are ω_{ν} and $|\omega_{\nu}\rangle$. The matrix elements

$$\langle j|V|k\rangle = \langle k|V|j\rangle^* = \xi_{jk}$$

are still assumed independent, identically distributed complex normal RVs

$$\langle \xi_{jk} \rangle = 0, \qquad \langle \xi_{jk}^* \xi_{mn} \rangle = v^2 \delta_{jm} \delta_{kn}$$
 (53)

We note the known fact that the ensemble of such random matrices V is invariant under all unitary transformations U, i.e. $U^{\dagger}VU \sim V$ [19]. Numerical simulations indicate that if $\Gamma := 2\pi\rho_0 v^2 \ll \Delta E$ and $\rho_0 \Gamma \gg 1$ then the DOS of H_1 is also ρ_0 , except near the endpoints of Δ .

Every eigenstate of H_0 will decay as a result of the interaction V. Numerical evidence indicates that the decay rate is near Γ when $\rho_0 \Gamma \gg 1$, and that the spectral densities are close to those found in Sect. 5. If this is true, then $|\langle k | \omega_v \rangle|^2$ inserted in (31) gives a spectral density near the Lorentz form, for every choice of k. (This fails for E_k near the end points of Δ , but we will argue as if $\Delta = \mathbb{R}$.) To justify this picture, pick any eigenvalue of H_0 that is not too close to the ends of Δ . Call it E_0 and calculate how the corresponding eigenstate $|0\rangle$ decays by transforming this problem into that already solved in Sect. 5. Make a decomposition

$$H_1 = H_{1A} + H_{1B} + V_1 + V_1^{\dagger}$$

where there is only one non-zero element of $H_{1A} = E_0 + \xi_{00}$, V_1 is defined by $(V_1)_{0k} := \xi_{0k}$ and what is left is H_{1B} . For each ξ in the ensemble (53) we can diagonalize H_{1B} by a unitary U which leaves the basis vector $|0\rangle$ invariant. The transformed Hamiltonian is

$$U^{\dagger}H_{1}U = H_{1A} + U^{\dagger}H_{1B}U + V_{1}U + U^{\dagger}V_{1}^{\dagger}$$

which is now of the form (21), where $H_A \rightarrow H_{1A}$ is 1-D, and $U^{\dagger}H_{1B}U$ is diagonal with eigenvalues randomly distributed, but with a level repulsion which makes the DOS nearly uniform and equal to ρ_0 on the average. Due to the unitary invariance of the ensemble (53), it holds that $V_1 \sim V_1 U$. Thus the solution in Sect. 5 will still hold here for the decay of the chosen state, with ρ_B replaced by ρ_0 . The fluctuation properties will also be the same.

It is also true that the phase transformations (a subgroup of the full invariance group)

$$V_{ik} \longrightarrow e^{i(\theta_j - \theta_k)} V_{ik}, \quad \theta_i \in [0, 2\pi)$$

leaves the ensemble (53) invariant. Under each such transformation the eigenvalues of (52) are invariant and the eigenvectors are just multiplied by a phase

$$\langle k | \omega_{\nu} \rangle \longrightarrow \mathrm{e}^{-i\theta_k} \langle k | \omega_{\nu} \rangle$$

Let $\zeta_k = \langle k | \zeta \rangle$ be the components of a vector. We can allow it to be a random vector, but assume it independent of the ensemble defined by (53). In the sum

$$\langle \zeta | \omega_{\nu} \rangle = \sum_{k} \zeta_{k} \langle k | \omega_{\nu} \rangle$$

an average over the ensemble (53), or just over all angles θ_k , gives zero, while in the average of the absolute square the cross terms vanish

$$\langle |\langle \zeta | \omega_{\nu} \rangle|^2 \rangle = \sum_k |\zeta_k \langle k | \omega_{\nu} \rangle|^2$$

Using the spectral density form (31) we find for $\rho_0 \Gamma \gg 1$

$$\langle |\langle \zeta | \omega_{\nu} \rangle|^2 \rangle \approx \rho_0^{-1} \sum_k \phi(\omega_{\nu} - E_k, \varepsilon) |\zeta_k|^2$$

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and replacing ζ_k by a smooth function $\zeta(E_k)$ and approximating by an integral

$$\langle |\langle \zeta | \omega_{\nu} \rangle|^2 \rangle \approx \int_{\mathbb{R}} dx \phi(\omega_{\nu} - x, \varepsilon) |\zeta(x)|^2$$

i.e. a convolution.

We now add another interaction term with the same distribution

$$H_2 = H_1 + V' = H_0 + V + V'$$

i.e. $V \sim V'$, but assume that V and V' are independent RVs. By the rules of adding independent normal RVs with zero mean $V + V' \sim \sqrt{2}V$. The diagonalization of H_2 can be done in one step using the interaction V + V', or in two, first making H_1 diagonal, then H_2 , while using the unitary invariance of the ensembles. Use $|\Omega_u\rangle$ for the eigenvectors of H_2 . Then expand the scalar product

$$\langle k | \Omega_u
angle = \sum_{
u} \langle k | \omega_
u
angle \langle \omega_
u | \Omega_u
angle$$

and average the absolute squared expression over all angles θ_k

$$\langle |\langle k | \Omega_u \rangle|^2 \rangle = \sum_{\nu} |\langle k | \omega_{\nu} \rangle|^2 |\langle \omega_{\nu} | \Omega_u \rangle|^2$$

Averaging over the angles only we need no averages in the RHS. Then approximate the sum by an integral, and replace the two factors by the spectral density ϕ_1 coming from diagonalizing H_1 starting from H_0 , and ϕ_2 coming from diagonalizing H_2 starting from H_1 . Finally we find the spectral density for diagonalizing H_2 starting from H_0 as a convolution

$$\phi(E_k - \Omega_u, 2\varepsilon) \approx \int dx \phi_1(E_k - x, \varepsilon) \phi_2(x - \Omega_u, \varepsilon)$$

With the explicit resonance form (40), we find that ϕ_1 and ϕ_2 have parameter Γ while that ϕ in the LHS has parameter 2Γ , coming from $V + V' \sim \sqrt{2}V$. Thus we recover (9) in the case $\Gamma_1 = \Gamma_2 = \Gamma$.

9 Higher Dimensions and Fano Lineshapes

We return to the Hamiltonian (21) and assume H_A to have a finite dimension $N_A > 1$. It can describe several states (interacting or not), all decaying into quasicontinua. In this case the decay depends strongly on the matrix elements of V; it is not always relevant to assume them all independent or with the same distribution as in (53). Pick one possible structure by choosing ξ to be complex, normal RVs defined by

$$\langle \xi_{jr} \rangle = 0, \qquad \langle \xi_{jr} \xi_{ks}^* \rangle = \gamma_{jk} \, \delta_{rs}$$

where γ is a positive semidefinite matrix of dimension $N_A \times N_A$. The imaginary part of (24) is then a positive semidefinite random matrix

$$G_{jk} := \left[\operatorname{Im} \tilde{H}_A(x - i\varepsilon) \right]_{jk} = \varepsilon \sum_r \frac{\xi_{jr} \xi_{kr}^*}{(x - E_r)^2 + \varepsilon^2}$$
(54)

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with ensemble average

$$\langle G_{jk} \rangle = \gamma_{jk} \varepsilon \sum_{r} \frac{1}{(x - E_r)^2 + \varepsilon^2} \approx \pi \rho_B \gamma_{jk}$$

Comparing with the case $N_A = 1$, it is natural to define the golden rule matrix

$$\Gamma_{jk} := 2\pi \rho_B \gamma_{jk} \tag{55}$$

The fluctuations around the average is estimated as in Sect. 6, and again found to contain a factor ω_B/ε , just like (41). Then (6) scales γ as $\gamma \to \lambda^2 \gamma$, and we will find the convergence to the ensemble mean in the limit $\lambda \to 0$ just as for $N_A = 1$. The same holds for Re \tilde{H}_A . Consequently the exponential solution (28) (including $\varepsilon = 0$) is justified.

When H_A and Γ commute and can be diagonalized simultaneously, each eigenstate decays independently and exponentially, each with a different Lorentz line shape and decay rate. When they do not commute, the present formalism includes models with Fano line shapes [7, 9, 10]. Assume that we can prepare the decaying system of N_A states in a definite quantum state $|\theta\rangle$. The lineshape function which will govern the non-exponential decay of this state is obtained from the spectral density (25) by projecting it on the corresponding 1-dimensional subspace (and setting $\varepsilon = 0$)

$$f(\theta, x) := \frac{1}{\pi} \langle \theta | \operatorname{Im} R_A(x) | \theta \rangle$$

Clearly the factor R_A in (25) will in general have N_A poles in the upper half plane (and R_A^{\dagger} the conjugate poles in the lower half plane); these poles will determine the spectral density, which is far from the simple Lorentz form in general. Depending on the vector $|\theta\rangle$ there will be a weighted interference of the contributions from the resonance poles. The standard Fano lineshapes can be reproduced for $N_A = 2$ by suitable choices of the parameters. When $N_A > 2$ the number of different possibilities increase rapidly.

10 Separation of Time Scales

In this section we will briefly analyze the deviations from exponential decay caused by a finite energy interval Δ or a finite DOS ρ_B . The conclusions have been compared to numerical simulations.

First consider the case when $\Delta = \mathbb{R}$ but $\rho_B < \infty$. When $\{E_k = k\omega_B; k \in \mathbb{Z}\}$, the "decay" is periodic with period $\tau_B := 2\pi\rho_B$. Clearly we need to have the decay time defined by Γ to be much shorter than that. This is so if $\omega_B \ll \Gamma$, or, equivalently $N_{\Gamma} \gg 1$. However, in order to find the time we need to see the deviation from an exponential decay to zero, another calculation is needed. Recall that $\Phi_A(x, 0)$ defined in (27) is a step function reflecting the discrete spectrum, but it still has a useful approximation (45). The decay (characteristic) function (26) will then be almost periodic. Consider the ergodic limit

$$\lim_{T\to\infty}\frac{1}{T}\int_0^T dt |\chi_A(t)|^2$$

For exponentially decaying amplitudes this is zero, but for a discrete nondegenerate spectrum the limit picks out conjugate Fourier coefficients of $\chi_A(t)$ and $\chi_A(t)^*$ reducing the

double sum to a single (diagonal) sum which is constant in time

$$\lim_{T \to \infty} \frac{1}{T} \int_0^T dt |\chi_A(t)|^2 \approx \frac{\omega_B^2 \Gamma^2}{(2\pi)^2} \sum_k \left[(E_s - E_k)^2 + \Gamma^2 / 4 \right]^{-2}$$

When the sum is approximated by an integral we find that

$$\lim_{T \to \infty} \frac{1}{T} \int_0^T dt |\chi_A(t)|^2 \propto \frac{\omega_B}{\Gamma} = \frac{1}{N_{\Gamma}}$$

Thus, over long times the function $|\chi_A(t)|^2$ is almost periodic, fluctuating around a non-zero mean value determined by N_{Γ} . We can expect to see the exponential decay in this fluctuating background only for *t* satisfying

$$t\Gamma < \ln N_{\Gamma} \tag{56}$$

Next we consider the effect of a finite ΔE while we can let $\rho_B = \infty$. Then $|\chi_A(t)|^2$ has a smooth quadratic maximum at t = 0. Numerical simulations for large values of ρ_B (taking into account the level shift) show that this function is close to an exponential for

$$t\Delta E \gg 1 \tag{57}$$

but they also indicate that there is a deviation from the exponential

$$|\chi(t)|^2 - \exp(-\Gamma t) = O(\Gamma/\Delta E)$$

which remains significant over a time interval of the order of $1/\Gamma$. When $\Gamma \ll \Delta E$ this deviation is very small, and the time $1/\Delta E$ is very short compared to the relaxation time scale. Then the effect of a finite ΔE on the relaxation will be insignificant, and the exponential is a good approximation.

Note that non-exponential decay for very long time scales due to a spectrum bounded below was discussed in [14].

11 Conclusions

In this paper we argue that the exponential relaxation and golden rule for Hamiltonians of the type (21) can be understood as fixed point properties of this class under a simple RG of transformations, e.g. in the form (49).

The mathematical basis for the results is the simple non-perturbative form (25) for the spectral density and the assumed uniformity of the spectrum of H_B and the matrix elements of V, for instance in terms of the relations (47) and (48). The method works for a single decaying state, with a simple Lorentzian lineshape, as well as more complex cases, including Fano lineshapes, and it does not involve an expansion in the coupling strength. Instead we estimated the deviations from the scaling limit when the scaling parameter λ is small but nonzero, and found that the deviation is small if the number of states under the resonance is large: $N_{\Gamma} = \rho_B \Gamma \gg 1$. We could also handle the case of a finite energy range ΔE for H_B . Using the dimensionless quantities N_{Γ} and $N = \rho_B \Delta E$ (the total number of states) the condition for small deviations (46) reads

$$1 \ll N_{\Gamma} \ll N$$

In Sect. 10 we concluded that the exponential decay is a very good approximation in a time interval restricted by (56) and (57). In terms of N and N_{Γ} we found that

$$N_{\Gamma}/N \ll t\Gamma < \ln N_{\Gamma}$$

In view of the frequent use of the van Hove limit (5) it is important to insist that (6) is not a weak coupling limit; instead it must be interpreted as a limit where the strength of the coupling is held constant while the reservoir is enlarged. In order to see this we first have to find a measure of the strength of the interaction term in Hamiltonian of Sect. 5. When $N_B < \infty$ then we can choose the square root of the positive scalar (expectation for a random V)

$$\langle VV^{\dagger}\rangle = N_B v^2 \approx \rho_B v^2 \Delta E = \frac{1}{2\pi} \Gamma \Delta E$$

to get a measure of dimension energy. In the scaling (6) the parameters Γ and ΔE are invariant, so is the strength of the interaction. When $\Delta E \rightarrow \infty$ this value is inevitably misleading. The matrix elements connecting the decaying level to off-resonant final states, i.e. with $|E_s - E_k| \gg \Gamma$, will have little influence on the decay except for very short or very long times. Provided $\Gamma \ll \Delta E$ we can then replace ΔE by a multiple of Γ and use the scaling invariant Γ itself as a useful measure of the strength of the interaction.

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References

- 1. Bixon, M., Jortner, J.: Intramolecular radiationless transitions. J. Chem. Phys. 48, 715 (1968)
- Carmeli, B., Nitzan, A.: Random coupling models for intramolecular dynamics. I. Mathematical approach. J. Chem. Phys. 72, 2054 (1980)
- Cohen-Tannoudji, C., Dupont-Roc, J., Grynberg, G.: Atom-Photon Interactions: Basic Processes and Applications. Wiley, New York (1992)
- 4. Cottle, R.W.: Manifestations of the Schur complement. Linear Algebra Appl. 8, 189 (1974)
- 5. Davies, E.B.: Markovian master equations II. Math. Ann. 219, 147 (1976)
- Derezinski, J., Früboes, R.: Fermi Golden Rule and open quantum systems. In: Attal, S., Joye, A., Pillet, C.A. (eds.) Lecture Notes in Mathematics, vol. 1882. Springer, Berlin (2006)
- Dietz, W., Fischer, S.F.: Line shape studies of a state coupled to a random background including large fluctuations of the couplings. J. Chem. Phys. 127, 094105 (2007)
- Dirac, P.A.M.: The quantum theory of emission and absorption of radiation. Proc. R. Soc. Lond. A 114, 243 (1927)
- 9. Durand, Ph., Paidarová, I., Gadéa, F.X.: Theory of Fano profiles. J. Phys. B 34, 1953 (2001)
- 10. Fano, U.: Effects of configuration interaction on intensities and phase shifts. Phys. Rev. 124, 1866 (1961)
- Feller, W.: An Introduction to Probability Theory and Applications, vol. 2, 2nd edn. Wiley, New York (1971)
- 12. Feshbach, H.: Unified theory of nuclear reactions. Ann. Phys. (N.Y.) 5, 357 (1958)
- 13. Feshbach, H.: A unified theory of nuclear reactions II. Ann. Phys. (N.Y.) 19, 287 (1962)
- Fonda, L., Ghirardi, G.C., Rimini, A.: Decay theory of unstable quantum systems. Rep. Prog. Phys. 41, 587 (1978)
- Freed, K.F.: Energy dependence of electronic relaxation processes in polyatomic molecules. Topics Appl. Phys. 15, 23 (1976)
- Jensen, A., Nenciu, G.: The Fermi golden rule and its form at thresholds in odd dimensions. Commun. Math. Phys. 261, 693 (2006)
- 17. Jona-Lasinio, G.: Renormalization group and probability theory. Phys. Rep. 352, 439 (2001)
- Löwdin, P.-O.: Studies in perturbation theory IV. Solution of eigenvalue problem by projection operator formalism. J. Math. Phys. 3, 969 (1962)
- 19. Mehta, M.L.: Random Matrices, 3rd edn. Elsevier, Amsterdam (2004)
- 20. Messiah, A.: Quantum Mechanics, vol. 2. North-Holland, Amsterdam (1962)

- Van Hove, L.: Quantum-mechanical perturbations giving rise to a statistical transport equation. Physica 21, 517 (1954)
- 22. Van Hove, L.: The approach to equilibrium in quantum statistics. A perturbation treatment to general order. Physica 23, 441 (1957)
- Weisskopf, V., Wigner, E.: Berechnung der natürlichen Linienbreite auf Grund der Diracschen Lichttheorie. Z. Phys. 63, 54 (1930)