Occurrence of exponential relaxation in closed quantum systems

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We investigate the occurrence of exponential relaxation in a certain class of closed, finite systems on the basis of a time-convolutionless projection operator expansion for a specific class of initial states with vanishing inhomogeneity. It turns out that exponential behavior is to be expected only if the leading order predicts the standard separation of time scales and if, furthermore, all higher orders remain negligible for the full relaxation time. The latter, however, is shown to depend not only on the perturbation (interaction) strength, but also crucially on the structure of the perturbation matrix. It is shown that perturbations yielding exponential relaxation have to fulfill certain criteria, one of which relates to the so-called "Van Hove structure." All our results are verified by the numerical integration of the full time-dependent Schrödinger equation.

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I. INTRODUCTION

A substantial part of linear nonequilibrium thermodynamics essentially relies on a description by means of rate equations, often in the form of master equations [1]. The crucial quantities, such as the probability to find the system in some state i,j or the amount of particles, energy, etc., at points i,j in some space, are routinely believed to follow equations such as

$$\frac{\partial}{\partial t}P_i = \sum_j R(j \to i)P_j - \sum_j R(i \to j)P_i \tag{1}$$

with time-independent transition rates from i to j, $R(i \to j)$. Pertinent examples are the decay of excitations in atoms, nuclear decay, etc. However, diffusive transport phenomena also belong to that class, since the diffusion equation can also be formulated to take the above form (random walk dynamics). Another implementation of that scheme is the (linear) Boltzmann equation [1,2], where particle scattering is taken into account by means of transition rates, and many more could be named.

However, regardless of the incontestable success of such descriptions, the strict derivation of rate equations from underlying principles often remains a problem. Typically, the descriptiveness by means of rate equations is taken for granted. Since those rate equations yield an exponential decay toward equilibrium, the basic question may be formulated as: How can an exponential decay of some observable be derived from the Schrödinger equation?

On the basis of quantum mechanics the most popular approach to this question is probably Fermi's Golden Rule [3]. Despite the undisputed descriptive success of this scheme, it is simply derived from first order perturbation theory, e.g., its validity generally breaks down on a time scale much shorter than the resulting relaxation time. Therefore it can hardly describe a complete decay into equilibrium. One of the few concrete, concise derivations of exponential decay is the Weisskopf-Wigner theory for the relaxation of excitations in an atom due to the coupling of the atom to a zero-temperature, broad-band electromagnetic field [4]. However, this theory is hardly generalizable, since it only applies if just one state is coupled to a multitude of others, rather than many states coupled to many others, as is typically the case.

A more abstract, rather fundamental approach has been suggested by Van Hove [5,6]. It is based on (infinite) quantum systems having continuous state densities and interactions which are described by smooth functions rather than discrete matrices. However, a lot of the findings for discrete systems in the paper at hand are quite parallel to Van Hove's, as will be pointed out below.

Other approaches are based on projection operator techniques, in particular the well-known Nakajima-Zwanzig (NZ) method. This method is commonly used in the context of open quantum systems, i.e., systems that allow for a partition according to a considered system (or simply "system") and an environment [1,7]. For a specific choice of the initial condition, as pointed out below, the projection onto the system's degrees of freedom eventually leads to an autonomous master equation describing the dynamics of the system, based on a systematic perturbation expansion. However, in general, due to the complexity of higher orders, only the leading order is taken into account. In the paper at hand we will demonstrate that this truncation may produce wrong results even and especially for the case of fast decaying correlation functions and arbitrarily weak interactions.

A further approach to this topic is based on the description of quasiparticle dynamics in many-particle systems by the use of Green's functions [8]. These considerations indicate the validity of a Boltzmann equation.

In the present paper we will employ another projection operator technique, the so-called time-convolutionless (TCL) method [9–14]. In the following we will follow the TCL method as detailed in Ref. [14]. In Sec. II we introduce our rather abstract Hamiltonian for a "closed quantum" system (consisting of an unperturbed part and a perturbation) and define an also rather abstract observable, the dynamics of which we are going to investigate. In Sec. IV we demonstrate how the TCL technique can be used to compute the above dynamics of the variable. (This is somewhat reminiscent of

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projection techniques using "correlated projectors" [15,16].) We tune our models such that a leading order truncation predicts exponential decay. For a "random interaction" this prediction turns out to be correct, as is verified by the numerically exact solution of the full time-dependent Schrödinger equation. In the following Sec. V nonrandom ("structured") perturbation matrices are discussed in more detail. While a leading order truncation still predicts exponential relaxation, it is demonstrated that this prediction may fail even for arbitrarily large models and arbitrarily small interactions. This breakdown stems from the fact that higher order contributions are not negligible if the interaction matrix violates certain criteria. Before we will close with a summary and conclusion in Sec. VI, these criteria will be also related to those conditions which Van Hove postulated in order to explain the occurrence of exponential relaxation.

II. MODELS, OBSERVABLES, AND INTERPRETATION OF DYNAMICS

In the present paper we will analyze quantum models which are much simpler than most of the examples mentioned in the Introduction. They are defined on a very general, rather formal level and are not meant to describe any specific, realistic quantum system in great detail. The Hamiltonian is taken to consist of a local part H_0 and an interaction part V such that $H=H_0+V$. In particular, V is assumed to take the special form of an "off-diagonal block structure" in the eigenbasis of H_0, that is, the matrix representation of H may be written as

$$H=\left(\begin{array}{cc|cc} \ddots & & 0 & \\ & \frac{i}{n-1}\delta\epsilon & & v \\ 0 & & \ddots & \\ \hline & & \ddots & 0 \\ & v^{\dagger} & & \frac{j}{n-1}\delta\epsilon \\ & & 0 & \ddots \end{array}\right) \tag{2}$$

or, equivalent to the above notation, $H=H_0+V$ may also be written as

$$H_0=\sum_{i=0}^{n-1}\frac{i}{n-1}\delta\epsilon|i\rangle\langle i|+\sum_{j=0}^{n-1}\frac{j}{n-1}\delta\epsilon|j\rangle\langle j|,$$

$$V=\left(\sum_{i,j=0}^{n-1}v_{ij}|i\rangle\langle j|+\text{H.c.}\right), \tag{3}$$

where $|i\rangle,|j\rangle$ form the basis in which Eq. (2) is represented. Obviously, the complete Hilbert space is divided into two subspaces, where i runs through the states of the first and j through the states of the second subspace, respectively. Obviously, H_0 may correspondingly be separated into two parts which we only specify very roughly at this point by two parameters: There are two identical "bands" with width $\delta\epsilon$ and n equidistant energy levels each.

The average strength of the interaction V is measured by

$$\lambda^2=\frac{1}{n^2}\sum_{i,j=0}^{n-1}|v_{ij}|^2. \tag{4}$$

In our first example in Sec. IV we take the matrix elements v_{ij} in the off-diagonal blocks to be Gaussian, complex, random numbers. For the other examples V will be specified below. In all cases the matrix elements of V in the diagonal blocks are all zero, just to keep the picture as simple as possible.

We will investigate the (relaxation) dynamics of an abstract observable a, represented by an operator A, which is chosen in such a way that

$$[A,H_0]=0,\text{Tr}\{A\}=0,\text{Tr}\{A^2\}=1. \tag{5}$$

The first of these properties states that A is diagonal in the eigenbasis of H_0, while the remaining two properties do not mean crucial restrictions on A. While all of the following will be correct for any A featuring the above properties, we mainly concentrate in our examples on "binary" operators, i.e., operators featuring only two different eigenvalues, namely, $+1/\sqrt{2n}$ in one subspace and $-1/\sqrt{2n}$ in the other. This means that $a\equiv\text{Tr}\{A\rho\}=+1/\sqrt{2n}$ indicates that the system entirely occupies one subspace and $a=-1/\sqrt{2n}$ indicates that it entirely occupies the other subspace. (Here, ρ is the density matrix for the state of the system.) If and only if $a(t)$ is found to relax exponentially to zero, the system allows for a merely statistical interpretation entirely beyond quantum physics: It is then in accord with a system featuring two distinguishable states in between it can "hop" with a given transition rate, the latter being equal for both directions. a then represents the difference between the probabilities of finding it in one or the other state, respectively.

In an abstract way the above model may represent many physical situations. It may be viewed as a simplified model for the exchange of an excitation between, e.g., two weakly coupled atoms, molecules, quantum dots, etc. A then represents the probability to find atom 1 excited, subtracted by the probability to find atom 2 excited, V represents the coupling in this scenario. Or it may model the momentum dynamics of a particle bound to one dimension which possibly changes its direction (forward-backward) due to some scattering. In a many-particle system the current operator could be identified with A and V may stand for a particle-particle interaction. This way the dynamics of the current autocorrelation function could be investigated based on the framework below. More detailed information about such models can be found in Refs. [17–22].

III. TCL SCHEME AND CHOICE OF THE PROJECTION OPERATOR

In this section we give a short overview of the time-convolutionless (TCL) projection operator technique [13,14]. Furthermore, we introduce the pertinent equations which are applied to models with various interactions in Secs. IV and V. A detailed derivation of these equations is beyond the scope of this paper and can be found in Refs. [14,20].

The TCL method is a projection operator technique such as the well-known NZ technique [23,24]. Both are applied in order to describe the reduced dynamics of a quantum system with a Hamiltonian of the type $H=H_0+V$. Generally, the full dynamics of the system are given by the Liouville–von Neumann equation

$$\frac{\partial}{\partial t}\rho(t) = -\imath[V(t),\rho(t)] = \mathcal{L}(t)\rho(t). \tag{6}$$

(Now and in the following all equations are denoted in the interaction picture.) In order to describe the reduced dynamics of the system, one has to construct a suitable projection operator $\mathcal{P}$ which projects onto the relevant part of the density matrix $\rho(t)$. $\mathcal{P}$ has to satisfy the property $\mathcal{P}^2\rho(t)=\mathcal{P}\rho(t)$. Recall that in our case the relevant variable is chosen as the expectation value $a(t)$ of the binary operator A. For initial states $\rho(0)$ with

$$\mathcal{P}\rho(0) = \rho(0) \tag{7}$$

the TCL method yields a closed time-local equation for the dynamics of $\mathcal{P}\rho(t)$,

$$\frac{\partial}{\partial t}\mathcal{P}\rho(t) = \mathcal{K}(t)\mathcal{P}\rho(t) \tag{8}$$

with

$$\mathcal{K}(t) = \sum_{i=1}^{\infty} \mathcal{K}_i(t). \tag{9}$$

The TCL technique avoids the usually troublesome time convolution which appears, e.g., in the context of the NZ technique. Equations (8) and (9) represent a formally exact perturbative expansion.

A brief comment on initial conditions should be made here. If Eq. (7) is not fulfilled, of course an additional inhomogeneity appears on the right-hand side of Eq. (8). This may change the solutions of Eq. (8) drastically, cf. Ref. [25], and references therein. However, for the model to be addressed below, there is substantial numerical evidence that, for a large set of initial states that do not fulfill Eq. (7), the dynamics are nevertheless reasonably well described by Eq. (8) (without inhomogeneity) [17,20,26–29]. Having mentioned this issue we consider in the following exclusively initial states in accord with Eq. (7).

For many models the odd cumulants of the expansion (9) vanish: $\mathcal{K}_{2i+1}(t)=0$. This will turn out to apply to our model as well. The lowest nonvanishing order scales quadratically with λ and reads

$$\mathcal{K}_2(t) = \int_0^t dt_1 \mathcal{P}\mathcal{L}(t)\mathcal{L}(t_1)\mathcal{P}. \tag{10}$$

For the fourth order term one finds

$$\begin{aligned}\mathcal{K}_4(t) = \int_0^t dt_1 \int_0^{t_1} dt_2 \int_0^{t_2} dt_3 & \mathcal{P}\mathcal{L}(t)\mathcal{L}(t_1)\mathcal{L}(t_2)\mathcal{L}(t_3)\mathcal{P} \\ & - \mathcal{P}\mathcal{L}(t)\mathcal{L}(t_1)\mathcal{P}\mathcal{L}(t_2)\mathcal{L}(t_3)\mathcal{P} \\ & - \mathcal{P}\mathcal{L}(t)\mathcal{L}(t_2)\mathcal{P}\mathcal{L}(t_1)\mathcal{L}(t_3)\mathcal{P} \\ & - \mathcal{P}\mathcal{L}(t)\mathcal{L}(t_3)\mathcal{P}\mathcal{L}(t_1)\mathcal{L}(t_2)\mathcal{P}. \end{aligned} \tag{11}$$

Note that the TCL approach is commonly used in the context of open quantum systems [1,14,23,24]. The TCL method is, however, also applicable to our closed quantum system.

To those ends, we define the projection operator $\mathcal{P}$ by

$$\mathcal{P}\rho(t) \equiv \frac{1}{2n}\hat{1} + A\mathrm{Tr}\{A\rho(t)\} = \frac{1}{2n}\hat{1} + Aa(t). \tag{12}$$

As already mentioned above, $\mathcal{P}$ is constructed to project onto the time-dependent expectation value $a(t)$ of the binary operator A, in the Schrödinger picture. However, since A commutes with H_0, this expectation value is identical in the interaction and the Schrödinger picture. The full dynamics [Hilbert space: dimension $2n$, Liouville space of density matrices: dimension $(2n)^2$] is broken down to the time evolution of the single variable $a(t)$, all other information is neglected. As a suitable initial condition we can then choose $\rho(0) = (1/2n)\hat{1} + (1/\sqrt{2n})A$ which implies $a(0)=1/\sqrt{2n}$. Inserting Eq. (12) into Eq. (8) yields the closed equation

$$\dot{a}(t) = \sum_{i=1}^{\infty} K_i(t)a(t) \tag{13}$$

with $K_i(t)=\mathrm{Tr}\{A\mathcal{K}_i(t)A\}$. Due to Eq. (12), the second order term reads

$$K_2(t) = -\int_0^t dt' C(t'), \tag{14}$$

where the two-point correlation function $C(t')$ is given by

$$C(t') = \mathrm{Tr}\{\imath[V(t),A]\imath[V(t_1),A]\}, \quad t' \equiv t - t_1. \tag{15}$$

A rather lengthy but straightforward calculation yields for the fourth order

$$\begin{aligned} K_4(t) &= \int_0^t dt_1 \int_0^{t_1} dt_2 \int_0^{t_2} dt_3\, I_1 + I_2 + I_3 + I_4, \\ I_1 &= \mathrm{Tr}\{[V(t_1),[V(t),A]][V(t_2),[V(t_3),A]]\}, \\ I_2 &= -C(t-t_1)C(t_2-t_3), \\ I_3 &= -C(t-t_2)C(t_1-t_3), \\ I_4 &= -C(t-t_3)C(t_1-t_2). \end{aligned} \tag{16}$$

IV. SECOND ORDER TCL AND COMPLETELY RANDOM INTERACTION

In this section we apply the equations in second order TCL to a model with the completely random interaction introduced in Sec. II. The function $C(t')$ in Eq. (15) is identical to the autocorrelation function of the interaction, since it can also be written as

$$C(t') = \frac{4}{n}\sum_{i,j=0}^{n-1} |v_{ij}|^2 \cos[\omega_{ij}(t-t_1)] \tag{17}$$

with frequencies $\omega_{ij}=(i-j)/(n-1)\delta\epsilon$ corresponding to H_0. Here, just as in many other examples, $C(t')$ decays within

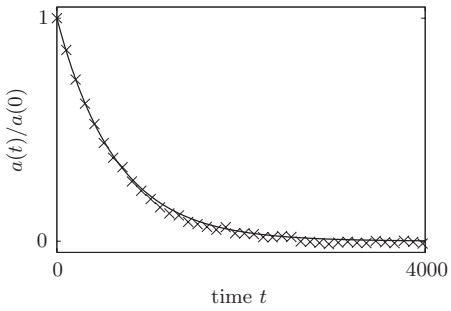

FIG. 1. Time evolution of the expectation value $a(t)$ for an interaction with completely random v_{ij}. The numerical result (crosses) indicates exponential behavior and is in very good agreement with the theoretical prediction (18) of second order TCL (continuous curve). The system parameters $n=1000$, $\delta\epsilon=0.5$, $\lambda=2.5\times10^{-4}$ fulfill the conditions (19).

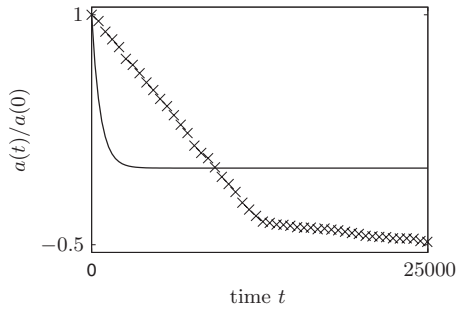

FIG. 2. Time evolution of the expectation value $a(t)$ for an interaction with $v_{ij}=\lambda$. The theoretical prediction (18) of second order TCL (continuous curve) fails to describe the numerical solution (crosses) correctly, although the system parameters $n=1000$, $\delta\epsilon=0.5$, $\lambda=2.5\times10^{-4}$ still fulfill the conditions (19). V violates the Van Hove structure.

the correlation time τ_C which is of the order of $\tau_C\approx4\pi/\delta\epsilon$ for our model. Afterwards the integral $K_2(t)$ becomes approximately time independent and assumes a constant value R until the "Heisenberg time" $T=2\pi n/\delta\epsilon$ is reached. This behavior can be inferred from integrating Eq. (17) and exploiting the properties of the sinc function. From this analysis also R may be found with an accuracy determined by the law of large numbers. Thus the second order approximation of Eq. (13) eventually results in

$$\dot{a}(t)=-Ra(t),\quad R\approx\frac{4\pi n\lambda^2}{\delta\epsilon}. \tag{18}$$

We hence obtain a rate equation featuring the form of Eq. (1) and thus exponential dynamics for $a(t)$. The solutions for $a(t)$ decay exponentially with a relaxation time $\tau_R=1/R$. However, this result is only valid within the boundaries $\tau_C\ll\tau_R<T$, because $K_2(t)$ can only be considered as time independent up to the Heisenberg time. Recall to this end that our model features equidistant energies such that $C(t')$ is strictly periodic with T. These two boundaries also result in two necessary criteria for the system parameters which have to be fulfilled in order to produce the occurrence of exponential dynamics

$$\frac{16\pi^2n\lambda^2}{\delta\epsilon^2}\ll1,\quad\frac{8\pi^2n^2\lambda^2}{\delta\epsilon^2}>1. \tag{19}$$

Remarkably, the whole derivation of the rate equation using second order TCL does not depend on the details of the interaction, i.e., the individual absolute values of the single matrix elements as well as their relative phases are not relevant. We should already mention here that the "structure," which we are going to introduce into the interaction in the following section, only concerns those details, hence the second order contribution K_2 will be the same in all our following examples.

In Fig. 1 the numerical solution of the Schrödinger equation is shown for the above repeatedly mentioned random interaction and compared with the TCL prediction. All parameters (the width of the Gaussian distribution according to which the matrix elements of V are generated, the bandwidth, etc.) are adjusted such that the criteria (19) are well satisfied. This solution is obtained by exact diagonalization. In fact, we find a very good agreement with the theoretical prediction of second order TCL.

V. FOURTH ORDER TCL AND NONRANDOM INTERACTIONS

In this section we will be concerned with the structure of the interaction matrix and, especially, its influence on the time evolution of the expectation value $a(t)$. It will be demonstrated that the theoretical prediction (18) of second order TCL fails to describe the numerically exact solution of the Schrödinger equation correctly for certain "interaction types," even and especially if the conditions (19) are fulfilled, i.e., the "strength" is "adequate." We will outline that this failure stems from the fact that the fourth order contribution of the TCL expansion is not negligible on the relaxation time scale which is obtained from second order TCL. However, the exact evaluation of $K_4(t)$ turns out to be almost impossible, analytically and numerically. Instead we will present feasible estimations of $K_4(t)/K_2(t)$ based on suitable approximations of $K_4(t)$ called $S(t)$ [see Eqs. (23) and (38)]. Whenever

$$q(t)\equiv\frac{S(t)}{K_2(t)}<1 \tag{20}$$

is violated the influence of higher order terms is not negligible. If this is the case for times t of the order of or shorter than τ_R, no exponential relaxation will result.

A. Uniform interactions and Van Hove structure

Let us start with an example. Figure 2 shows the time evolution of the expectation value $a(t)$ for an interaction with $v_{ij}=\lambda$. This type of interaction is, of course, highly nonrandom, since all matrix elements have the same absolute value and phase. The second order approximation obviously yields a wrong description for this interaction structure, that is, the dynamics are not exponential, although both of the conditions (19) are well fulfilled. It should be remarked again that

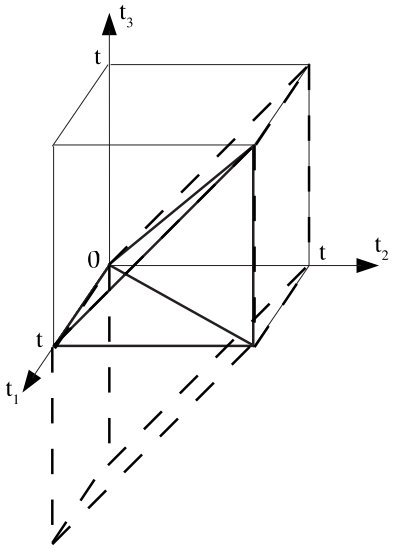

FIG. 3. Sketch for the integration volume of $K_4(t)$ for fixed t. The cube with the edge length t is drawn with thin lines, the actual integration volume is marked with thick lines. The dashed lines represent the changed integration volume which is used in the approximations.

the observed nonexponential behavior definitely is a structural issue. For instance, it cannot be "repaired" by simply decreasing the overall interaction strength, because this decrease would eventually lead to the violation of the criteria (19).

To analyze this model we now develop our first estimate $S(t)$ for $K_4(t)$ which concerns the time scale $t > \approx \tau_C$. We start from Eq. (16), where we abbreviate the triple time integration by a single "$\int$." One may hence write $K_4(t) = \int I_1 + I_2 + I_3 + I_4$. Figure 3 shows a sketch for the integration volume of $K_4(t)$ in the three-dimensional space which is spanned by t_1, t_2, t_3. The integration does not run over the whole cube with the edge length t, but only over the region where $t_3 \leq t_2 \leq t_1$ holds.

$C(t-t_1)$ is the autocorrelation function of the interaction which has already been mentioned in Eq. (15). Recall that $C(t')$ is only different from zero around $t'=0$ in a small interval of the width τ_C. Thus, the integrands I_2, I_3, I_4 are only different from zero in a small volume around the region where both of the arguments are equal for each of the two multiplied correlation functions.

First of all let us focus on I_3 as well as I_4. The integrand I_3 contributes to $K_4(t)$ for $t=t_2$ and $t_1=t_3$, while the integrand I_4 contributes to $K_4(t)$ for $t=t_3$ and $t_1=t_2$, respectively. The sketch in Fig. 3 displays that both of these regions overlap only in the vicinity of one single point with the integration volume of $K_4(t)$, namely, at the point where all arguments are equal to t. Especially, this overlap does not increase with t. Therefore the triple time integration is estimated by $\int I_3 \approx \int I_4 \approx C(0)^2 \tau_C^3$. Using the estimate $R \approx C(0)\tau_C$, we eventually obtain for the ratio between the contributions from I_3, I_4 to the fourth order and the second order $K_2(t > \tau_C)$ for times $t > \tau_C$

$$\frac{\int I_3}{R} \approx \frac{\int I_4}{R} \approx C(0)\tau_C^2 \approx \frac{\tau_C}{\tau_R} \equiv \alpha. \tag{21}$$

Recall that the derivation of exponential behavior within second order TCL has required $\tau_C \ll \tau_R$ or, equivalently, $\alpha \ll 1$ such that the contributions to $K_4(t)$ which arise from I_3 and I_4 are negligible, at least in comparison with R.

Analogous conclusions cannot be made for the term I_2, because its overlap with the integration volume is larger and grows with t. We have to find another estimation for the contributions of I_2 as well as I_1, of course. Our estimation is based on the fact that neither I_2 nor I_1 can decay on a shorter time scale than τ_C in any possible direction of the (t_1, t_2, t_3) space. This fact is obviously correct for I_2. But what about I_1? Since the term I_1 consists of summands which have the typical form

$$v_{ab} v_{bc} v_{cd} v_{da} e^{-\imath \omega_{ab} t} e^{-\imath \omega_{bc} t_1} e^{-\imath \omega_{cd} t_2} e^{-\imath \omega_{da} t_3}, \tag{22}$$

only those frequencies and, especially, those largest frequencies in I_1 which have already appeared in $C(t')$ contribute significantly to I_1. Consequently, I_1 can never decay faster than $C(t')$ in any possible direction of the (t_1, t_2, t_3) space. In the (possibly unrealistic) "best case" $I_1 + I_2$ decays within τ_C around the point $I_{1/2}(t,t,t,t) = I_{1/2}(0,0,0,0) \equiv I_{1/2}(0)$. We can therefore estimate the value of $q(\tau_C)$ by

$$\frac{\int I_1 + I_2}{R} \approx \frac{[I_1(0) - C(0)^2]\tau_C^3}{C(0)\tau_C} = \left[\frac{I_1(0)}{C(0)^2} - 1 \right] \alpha \equiv \beta. \tag{23}$$

β is a lower bound for the ratio between the fourth and the second order of TCL for times $t > \tau_C$. If $\beta \approx 1$ or even larger, then $K_4(t > \tau_C)$ dominates $K_2(t > \tau_C)$, that is, exponential behavior in terms of the second order prediction cannot occur. $\beta \ll 1$, however, does not allow for a strict conclusion, since a slower decay of I_1 or I_2, as the case may be, raises their contribution to $K_4(t)$. Nevertheless, the condition $\beta \ll 1$ is an additional criterion for the occurrence of exponential decay which involves the structure of V.

In the following we will discuss why and to what extend β and, especially, the ratio $I_1(0)/C(0)^2$ is related to the conditions which have been postulated by Van Hove for the interaction V in order to explain the onset of exponential relaxation, see Refs. [5,6]. To this end, let us define a Hermitian operator G by

$$G \equiv [V,[V,A]]. \tag{24}$$

A straightforward calculation yields

$$I_1(0) = \mathrm{Tr}\{G^2\} = \sum_{i,j} |G_{ij}|^2, \quad C(0) = \mathrm{Tr}\{AG\}, \tag{25}$$

where G_{ij} represents the matrix elements of G in the eigenbasis of H_0. Furthermore, let us also introduce the superoperator $\mathcal{D}$ which is given by

$$\mathcal{D}M \equiv \sum_i |i\rangle M_{ii} \langle i| \tag{26}$$

and projects any operator M onto its diagonal elements in the eigenbasis of H_0. Then the expression

$$(A,G) \equiv \mathrm{Tr}\{A\mathcal{D}G\} \tag{27}$$

defines an inner product between the operators A and G, because $(A,G)=(G,A)^*[=(G,A)]$ holds and $(A,A)=1$, as well as $(G,G)=\Sigma_i G_{ii}^2$, are both positive, real numbers. The Schwartz inequality $(A,G)^2 \leq (A,A)^2(G,G)^2$ can consequently be formulated. By the use of $(A,G)=C(0)$ we eventually obtain

$$C(0)^2 \leq \sum_i G_{ii}^2 \leq \sum_{i,j} |G_{ij}|^2 = I_1(0), \tag{28}$$

i.e., $I_1(0)/C(0)^2 \geq 1$. $C(0)^2$ is at most as large as the sum of the squared diagonal elements of G, according to the above equation. Therefore $I_1(0)/C(0)^2 \approx 1$ and hence sufficiently small β can only be realized if the diagonal elements of G and thus the diagonal elements of V^2 are as large as possible in comparison with the remaining nondiagonal elements of V^2 (G). In principle, this is essentially what Van Hove proclaimed [5,6].

In this sense, we define the "Van Hove structure" in the context of finite quantum systems: The interaction V is said to feature Van Hove structure if

$$\beta' \equiv \frac{I_1(0)}{C(0)^2}\alpha \ll 1, \tag{29}$$

while all conditions of second order TCL are simultaneously kept, of course. The latter refers to the validity of Eq. (19). The comparison with Eq. (23) shows that the Van Hove structure implies $\beta \ll 1$ and hence the relaxation may possibly be exponential, as described by the second order. Since the evaluation of β' is much more efficient than the complete computation of fourth order TCL [there is no time dependence left, e.g., $I_1(0)$ only depends on $t=t_1=t_2=t_3=0$], the Van Hove structure eventually is an assessable criterion for the possible occurrence of exponential decay. It is a criterion in the sense that only if Eq. (29) is satisfied, a use of the second order approximation is justified for any time longer than the correlation time, i.e., $t > \tau_C$.

Let us now apply these results to the already introduced models with random and nonrandom $(v_{ij}=\lambda)$ interactions, respectively. The only term which varies for the different models is $I_1(0)$, since the terms $C(0)^2 \approx n^2\lambda^4$ and $\alpha \approx 16\pi^2 n\lambda^2/\delta\epsilon^2$ (again with an accuracy set by the law of large numbers for the random interaction) are the same for random and nonrandom interactions. For the random interaction a straightforward calculation leads to

$$I_1(0) = 32n^2\lambda^4, \quad \beta' = 2\alpha \ll 1 \tag{30}$$

such that the random interaction indeed features Van Hove structure. This agrees with the numerical results in Fig. 1 which yielded exponential relaxation. In the case $v_{ij}=\lambda$, however, we finally obtain

$$I_1(0) = 16n^3\lambda^4, \quad \beta' = \frac{16\pi^2 n^2\lambda^2}{\delta\epsilon^2}, \tag{31}$$

where $\beta' > 1$, according to Eq. (19). The absence of the Van Hove structure already suffices to explain the breakdown of exponential behavior in Fig. 2.

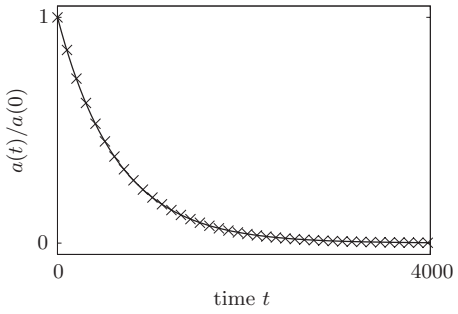

FIG. 4. Time evolution of the expectation value $a(t)$ for the interaction of spin-boson type. The numerical result (crosses) indicates exponential behavior and perfectly agrees with the theoretical prediction (18) of second order TCL (continuous curve). System parameters: $n_1=1$ (single level), $n_2=2000$ (many levels), $\delta\epsilon=0.5$, $\lambda=2.5\times10^{-4}$.

One may nevertheless be inclined to argue that the Van Hove structure is not the crucial difference between those two cases but simply the randomness of the matrix elements (which possibly induces quantum chaos). We therefore present a counterexample which immediately disproves such an argument. The example is slightly different from the others, since the complete system is not partitioned into equally large subspaces. n_1 and n_2 define the number of levels of the respective subspaces. One subspace consists of only one state $(n_1=1)$. Thus, in the matrix V there is only a single column with nonzero elements and a single row, respectively. Although these nonzero elements are chosen to be all equal (nonrandom), it can be shown that this V features Van Hove structure. Note that such a Hamiltonian occurs, e.g., in the context of spin-boson models at zero temperature or the scenario addressed by the Weisskopf-Wigner theory, see Ref. [14].

Figure 4 shows an almost perfect correspondence between the numerical solution of the Schrödinger equation and the theoretical prediction (18) which is obtained by the use of second order TCL. Here, exponential relaxation is found, although V is not randomly chosen.

B. Sparse interaction and localization

So far, we numerically found exponential decay in accord with the second order for all considered models that showed the Van Hove structure. There is, however, nonexponential behavior for some types of interactions which feature the Van Hove property in the sense of Eq. (29) and are in accord with Eq. (19). Recall that those are only necessary but not sufficient conditions for the occurrence of exponential decay.

An example for such a situation is a model with a random but, say, "sparsely populated" interaction. This model is almost identical to the model with the completely random interaction. The only difference is that only 1/10 of the matrix elements are Gaussian distributed numbers, all others are zero. The nonzero numbers are randomly placed. Apparently, this type of interaction fulfills the Van Hove structure, since the completely random interaction already does.

Figure 5 displays the numerical solution of the Schrödinger equation and the theoretical prediction (18) of

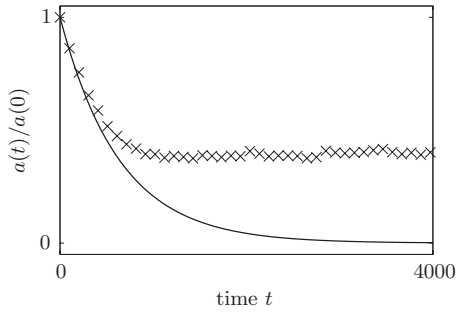

FIG. 5. Time evolution of the expectation value $a(t)$ for an interaction with random but "sparsely populated" v_{ij}. The theoretical prediction (18) of second order TCL (continuous curve) deviates from the numerical solution (crosses), even though the Van Hove structure as well as the conditions (19) are fulfilled. System parameters: $n=1000$, $\delta\epsilon=0.5$, $\lambda=2.5\times10^{-4}$.

second order TCL. At the beginning there is a good agreement but then the numerical solution starts to deviate from a purely exponential decay and finally sticks at a clearly positive value. The latter nonzero value may be a hint toward localization effects which also appear, e.g., in the context of the Anderson model [30–33]. And in fact, the sparsely populated interaction takes a form which is very similar to the Hamiltonian of the, e.g., three-dimensional Anderson model in the chaotic regime.

Apparently, we have to extend the analysis of the fourth order: There is no exponential behavior by the means of a complete exponential decay, although V fulfills the Van Hove property. Recall that the Van Hove criterion has been derived from the consideration of times $t<\approx\tau_C$ and thus $t=t_1=t_2=t_3<\approx\tau_C$. Hence, we have to reconsider the full time dependence of the fourth order to produce a feasible estimate for the time scale $t\approx\tau_R$. To this end, the integrand I_1 is expressed by

$$I_1 = \mathrm{Tr}\{G(t_1,t)G(t_2,t_3)\}, \tag{32}$$

where the Hermitian operator $G(t_1,t)$ is again given by

$$G(t,t_1) \equiv [V(t),[V(t_1),A]]. \tag{33}$$

If $I_1(0)\approx C(0)^2$, the diagonal terms dominate at $t=t_1=t_2=t_3$. Based on this fact, we carefully assume that I_1 is dominated by these terms for other times as well. Of course, this assumption neglects the larger part of all terms but leads, as will be demonstrated below, to a criterion which may be evaluated with limited computational power. (For our simple example its validity can also be counterchecked by direct numerics.) However, following this assumption, I_1 can be approximated by

$$I_1 \approx \sum_i G_{ii}(t-t_1)G_{ii}(t_2-t_3), \tag{34}$$

where $G_{ii}(t-t_1)$ are the diagonal matrix elements of $G(t,t_1)$ in the eigenbasis of H_0, namely,

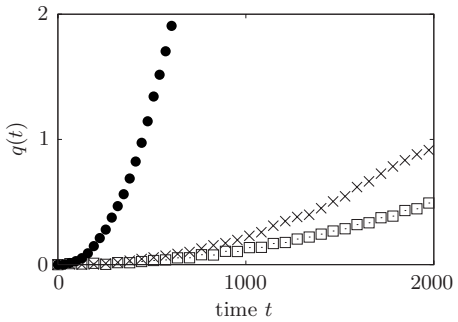

FIG. 6. Time evolution of the value $q(t)$ based on Eq. (38). $q(t)$ is numerically calculated for a completely random interaction (crosses), the interaction of spin-boson type (squares), and the random but sparsely populated interaction (circles). Note that $K_2(t)$ is a constant which is also identical for all three interactions. The system parameters are chosen according to Figs. 1, 4, and 5, respectively.

$$G_{ii}(t-t_1) = 2\sum_j (A_{ii}-A_{jj})|V_{ij}|^2\cos[\omega_{ij}(t-t_1)]. \tag{35}$$

Furthermore, the correlation function $C(t-t_1)$ can, by the use of this notation, also be written as

$$C(t-t_1) = \sum_i A_{ii}G_{ii}(t-t_1) \tag{36}$$

such that I_2, the remaining fourth order integrand, can be expressed as well by

$$I_2 = -\sum_{i,j} A_{ii}G_{ii}(t-t_1)A_{jj}G_{jj}(t_2-t_3). \tag{37}$$

In order to estimate with reasonable computational effort how $K_4(t)$ compares with $K_2(t)$ another approximation is necessary. Obviously, the expressions for I_1, I_2 are invariant along lines described by $t_1=\text{const}$, $t_2=t_3$. Thus, as an approximation, we shift the integration volume from the original region, indicated with solid lines in Fig. 3, to a new region, indicated with dashed lines in Fig. 3. Obviously, this is a rather rough estimate but it will turn out to be good enough for our purposes. Now the coordinate transformation $x=t-t_1$, $y=t_2-t_3$, $z=t-t_2$ decouples the integrations within the new integration volume such that we eventually find for $S(t)\approx K_4(t)$ (if V features Van Hove structure)

$$S(t) = t\left[\sum_i \Gamma_i(t)^2 - K_2(t)^2\right], \tag{38}$$

with the time integral $\Gamma_i(t)\equiv\int_0^t dt' G_{ii}(t')$. Now Eq. (20) may eventually be checked with very low computational power, based on $S(t)$ from Eq. (38). This adds to Eqs. (19) and (29) as a further manageable criterion for exponential relaxation. Figure 6 shows $q(t)$ [based on Eq. (38)] for the following interaction types: the completely random interaction, the interaction of spin-boson type, and the random but sparsely populated interaction. Figure 6 apparently demonstrates that this approximation is able to explain the breakdown of exponential behavior in the case of a random, sparsely populated interaction: The fourth order becomes roughly as large as the second order at a time which agrees with the deviation

between the second order theory and the numerical results in Fig. 5. In both other cases $q(t)$ remains sufficiently small, at least until the relaxation time is reached.

Obviously, regardless of the interaction type $K_4(t)$ will eventually dominate $K_2(t)$ for large enough times (cf. Ref. [34]). This, however, does not necessarily spoil the exponential decay: If $a(t)$ has already decayed almost completely into equilibrium, even a significant change of the rate $K(t)$ will not change the overall picture of an exponential decay [as long as $K(t)$ remains negative]. The influence of a large $K_4(t)$ will only be visible if it occurs, while $a(t)$ is still far from equilibrium, i.e., at times of the order of τ_R. If one now computes the ratio $q(t)$ for the time $t=\tau_R$, one finds

$$q(\tau_R) \approx \frac{\sum_i \Gamma_i(\tau_R)^2}{R^2} - 1, \tag{39}$$

where one has to take Eq. (38) and $K_2(\tau_R)=R=1/\tau_R$ into account. This form has the advantage of being completely independent of the overall interaction strength λ. One can hence compute $q(\tau_R)$, taking τ_R as a free variable. The region in which $q(\tau_R)<\approx 1$ then represents the range of different τ_R for which exponential decay is possible and to be expected. The different "possible" τ_R can then be implemented by tuning λ appropriately. Often $q(\tau_R)$ is found to increase monotonously, essentially as in Fig. 6. Thus a good number to characterize a class of models with different relaxation times (interaction strengths) would be $\tau_{\max}$ as the largest time for which $q(\tau_{\max})<\approx 1$ holds true. This then indicates the largest timescale on which exponential relaxation can still be expected. We should note here that we intend to use this measure $\tau_{\max}$ to investigate transport behavior in models of the Anderson-type in a forthcoming paper.

VI. SUMMARY AND OUTLOOK

We investigated the dynamics of some expectation values for a certain class of closed, finite quantum systems by means of the TCL projection operator method. This technique yields a perturbation expansion for those dynamics. Taking only the second (leading) order into account, we find that the evolution of these expectation values may be described by a rate equation, i.e., they relax exponentially if certain criteria are fulfilled. Those criteria, however, only depend on "rough" parameters such as overall interaction strength, bandwidth, and density of states but not on, e.g., the phases of the interaction matrix elements. An adequately computed numerical solution of the Schrödinger equation is in accord with this leading order result for random interaction matrices. However, numerics also show that this accordance breaks down if one considers nonrandom interactions, even if the above rough criteria are met. This, of course, indicates that higher orders are not negligible, depending on the structure, not only on the strength of the interaction. Subsequently, we established a numerically simple estimate for the absolute value of the fourth, i.e., the next higher order, in comparison to the second, for short times. From this approach it can be inferred that the fourth order remains negligible at small times if the interaction features a certain structure which we define as Van Hove structure according to Ref. [5]. However, numerics indicate that for certain interaction structures the fourth order may become non-negligible at larger times, thus spoiling the exponential relaxation, even if the interaction features Van Hove structure. Hence we suggest one more criterion [based on Eqs. (20) and (38)] that allows for the detection of such a behavior without diagonalizing the full system.

Diffusive transport in spatially extended quantum systems may be viewed as a form of exponential relaxation. Thus we intend to exploit the various criteria which are suggested in this paper to investigate the occurrence of diffusion in the Anderson model and/or other solid state models that do not allow for a full numerical diagonalization.

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