Influence functionals: General methodology for subsystem calculations

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Feynman path integrals offer a convenient and elegant tool for dealing with the statistical physics of quantum-mechanical systems. By using the Trotter product formula, one can evaluate directly the propagation of many-body quantum systems in imaginary time. The idea of an influence functional arises when one wishes to consider division of the physical system into a primary system and a bath. We present a general approach to the problem of constructing influence functionals, one that is capable of dealing both with Boltzmann baths (classical oscillators) and quantum baths of bosons or fermions. The fermion bath of special interest is generally a submanifold of the electronic state such as the bridge structure connecting chromophores or electron localization subunits which are common in problems of mixed valency and superexchange. The fermion bath is treated by a general rewriting of the influence phase S as a sum of an eigenvalue part S_{EV} and a remainder, S^0, that describes transitions. Reduction of the original Hamiltonian leads to a reduced Hamiltonian with effective off-diagonal matrix elements and influence functionals which can include memory effects. We present a general formalism for construction of influence functionals, and discuss particular applications to systems of interest, especially in electronic-structure problems. The following paper presents a variational technique for finding effective Hamiltonians.

I. INTRODUCTION

There are many physical problems in which only a small number of states is required to describe quite completely the energetics and/or dynamics; examples include coupled spins, minimum-basis electronic-structure models, and angular momentum systems. More generally, however, one is interested in situations in which attention is focused on a subsystem of a larger system that contains a very large (perhaps infinite) number of states. Examples include an atom or molecule interacting with a solvent, impurity levels in solids, chromophore subunits of large molecules, optically strong vibrational levels in a far larger overall vibrational problem, adsorbates on solid surfaces, and colloidal particles in a host. For all of these systems, solution via diagonalization of a large matrix representation is impractical; rather one would like to obtain a proper technique for describing the subsystem of primary interest, with proper consideration of the secondary states. One powerful technique for studying such influence problems includes the use of Feynman path-integral methods,[1] in which influence functionals characterize the effect of the secondary manifold of states.

Influence functionals provide a method to deal with degrees of freedom which are known either precisely or only statistically.[2(a)] A standard model is the influence functionals for a harmonic bath.[2(b)] The great advantage of this functional comes from the fact that it leads just to Gaussian integrals and these can be handled very easily. An alternative (non-Gaussian) influence functional was constructed by Soper.[3] Our aim here is to extend a method introduced in Ref. 4(a) to derive a general class of influence functionals for a decomposition of a Hamiltonian. Starting from a mathematical point of view, we obtain a very useful tool for a large variety of problems. It even contains the idea of an influence functional dealing simultaneously with the effects of a harmonic bath *and* of a fermionic bath.

We give the basic idea in Sec. II and derive from this a general formula for the evaluation of influence functionals. Further, we discuss some connections to known theories like the influence functional for a harmonic bath or a bath of two-level systems.[4(b)] In Sec. III we create some algebraic techniques to make the basic theory applicable. We work out two fundamental properties of transitions of a system and discuss the connection with symmetry properties. An important eigenvector property of constant paths is investigated; this facilitates the separation of the overall influence functional into an eigenvalue part characterizing propagation in given eigenfunction space and a remainder, characterizing transitions. In Sec. IV we evaluate three straightforward, but realistic examples in order to demonstrate the characteristics of the application of the evaluated mathematics. Section V embeds the harmonic-bath idea in our formalism, and presents a discussion of the harmonic bath, that will be extended in the following paper.[5] In Sec. VI we finally construct the influence functionals for two general examples explicitly and describe the main features. The following paper contains variational techniques for the general construction of influence functionals, based on the formalism developed here.

II. GENERALIZED PATH INTEGRALS AND INFLUENCE FUNCTIONALS

A. Basic theory

Path integrals are a special tool for evaluating propagators, i.e., exponential functions of Hamiltonians, using

Trotter's product formula.[6] This formula shows that a propagator can be calculated by multiplying its first-order short-time expansion so often that the sum of the short times is just a given time. The essential physical idea is that one gets the same result if one propagates a system in time all at once or if one breaks the time in arbitrary slices and propagates the system one time slice after the other. We are especially interested in statistical properties of a quantum system and therefore always work in imaginary times $\beta\hbar \equiv \hbar/kT$. Time slices are denoted throughout the presentation by $\epsilon\hbar \equiv \beta\hbar/P$, where P is a large natural number, the number of time slices used. If one has written a time propagator of a given system as a product of short-time propagators and one tells how to perform these operator products, namely, by inserting a resolution of the identity in some basis between every single product, than a usual path-integral representation of the propagator is obtained.[7] The generalization of path integrals in imaginary time that we will employ arises from the fact that one can calculate with blocks of a block-decomposed matrix precisely as with matrix elements, in the sense that a square or any power of a block-decomposed matrix is evaluated by summing up products of blocks in the same manner as one does with matrix elements evaluating matrix products.

We start our theory very formally by defining a block decomposition of a given Hamiltonian. Equivalently, we first define a resolution of the identity of a given Hilbert space $\mathbb{H}$, called the original system space; let K_i, $i=1,2,\ldots,N$ be a complete set of orthogonal projectors operating on $\mathbb{H}$. Then we can write the Hilbert space $\mathbb{H}$ as a direct sum of the subpaces[8] $\mathbb{H}_i \equiv K_i(\mathbb{H})$,

$$\mathbb{H} = \oplus_{i=1}^{N} \mathbb{H}_i \ . \tag{1}$$

N might be a natural number or infinity. Let now $H(\tau)$ be an arbitrary Hamiltonian on $\mathbb{H}$ dependent on the imaginary time τ. The imaginary-time variable τ runs of course between 0 and $\beta\hbar$. The number P of time slices $\epsilon\hbar$ is assumed to be large in the sense that Trotter's product formula can be applied to the imaginary-time propagator of H using a first-order expansion of the short-time propagator of H in ϵ:

$$\begin{aligned} &\exp\left[-\frac{1}{\hbar}\int_0^{\beta\hbar} H(\tau)d\tau\right] \\ &= \prod_{\alpha=0}^{P-1} (Id - \epsilon H^{(\alpha)}) \\ &= \sum_{b^{(0)},\ldots,b^{(P)}=1}^{N} \prod_{\alpha=0}^{P-1} K_{b^{(\alpha)}} e^{-\epsilon H^{(\alpha)}} K_{b^{(\alpha+1)}} \end{aligned} \tag{2}$$

with the abbreviation $H^{(\alpha)} \equiv H(\alpha\epsilon\hbar)$ for $\alpha = 0,1,\ldots,P$. The operator product is understood to be time ordered. The operators in the last line of Eq. (2) are mappings between the subspaces $\mathbb{H}_i$ of $\mathbb{H}$ and therefore represent a block decomposition of the Hamiltonian H. We obtained a generalized path integral for the propagator of H. Given the propagator of a system one can by definition calculate the thermal-equilibrium average of any Hermitian operator L on $\mathbb{H}$ by

$$Q(\beta)\langle L\rangle_{\text{equ}} = \text{Tr}\left[\exp\left[-\frac{1}{\hbar}\int_0^{\beta\hbar} H(\tau)d\tau\right] L\right] , \tag{3}$$

where $Q(\beta)$ denotes the partition function of H and Tr the trace operator. But a path-integral representation of the propagator as in Eq. (2) has an advantage only if we can solve the path integral, at least together with the trace operator in Eq. (3); the usefulness of the concept arises from success in evaluation, not just from rewriting. Whereas the purely theoretical part of this paper is also true for real time, we restrict the treatment to imaginary time when we discuss variational solutions of the path integral. These variational techniques are very effective but applicable to imaginary time only.

Generally we like to treat the path integral by reducing the system space $\mathbb{H}$ to a (smaller) space $\overline{\mathbb{H}}$ of dimension N. We call $\overline{\mathbb{H}}$ the reduced system space. Further, we assume an orthonormal basis of vectors $|\bar{i}\rangle$, $i=1,\ldots,N$, which spans the reduced system space $\overline{\mathbb{H}}$. If N is finite we can take without loss of generality $\overline{\mathbb{H}} = \mathbb{C}^N$ and $|\bar{i}\rangle$, the ith unit vector of $\mathbb{C}^N$. To the Hamiltonian $H^{(\alpha)}$ defined on the original system space $\mathbb{H}$ we associate now a Hamiltonian $\overline{H}^{(\alpha)}$ operating on the reduced system space $\overline{\mathbb{H}}$ so that for all α and for all $i \neq l$ the following condition is fulfilled:

$$\langle \bar{i} \,|\, \overline{H}^{(\alpha)} \,|\, \bar{l}\rangle = 0 \Longleftrightarrow K_i H^{(\alpha)} K_l = 0 \ . \tag{4}$$

For the rest, $\overline{H}$ is for the moment left arbitrary. The path sum equation (2) can of course be considered as a path sum in the reduced space $\overline{\mathbb{H}}$ because the labels have values between 1 and N. It is now most important for the formal part of the theory to express the original short-time propagators by reduced short-time propagators and an influence from the reduction. With the shorthand notation for the matrix elements of the reduced Hamiltonian $\overline{H}$,

$$\bar{h}_i^{(\alpha)} \equiv \langle \bar{i}|\overline{H}^{(\alpha)}|\bar{i}\rangle, \quad \bar{t}_{i,l}^{(\alpha)} \equiv \langle \bar{i}|\overline{H}^{(\alpha)}|\bar{l}\rangle \quad \text{for } i \neq l \ , \tag{5}$$

we define block operators from the original Hamiltonian H by

$$H_i^{(\alpha)} \equiv K_i H^{(\alpha)} K_i - \bar{h}_i^{(\alpha)} K_i, \quad T_{i,l}^{(\alpha)} \equiv K_i H^{(\alpha)} K_l / \bar{t}_{i,l}^{(\alpha)} \tag{6}$$

if $\bar{t}_{i,l}^{(\alpha)} \neq 0$. If $\bar{t}_{i,l}^{(\alpha)}$ vanishes we choose $T_{i,l}^{(\alpha)}$ arbitrary. Further, we set for notational convenience for equal indices $T_{i,i}^{(\alpha)} \equiv K_i$. Note that $H_i^{(\alpha)}$ is a Hamiltonian on the subspace $\mathbb{H}_i$ of $\mathbb{H}$ whereas the operators $T_{i,l}^{(\alpha)}$ are dimensionless. With these definitions the following basic observation connects the short-time expansions of the original and the reduced propagators:

$$K_i e^{-\epsilon H^{(\alpha)}} K_l = \langle \bar{i}|e^{-\epsilon \overline{H}^{(\alpha)}}|\bar{l}\rangle T_{i,l}^{(\alpha)} K_l e^{-\epsilon H_l^{(\alpha)}} K_l \ . \tag{7}$$

The first factor is a complex number and therefore commutes with all the operators. Inserting the factorization Eq. (7) in the path sum formula Eq. (2) we obtain

$$\exp\left[-\frac{1}{\hbar}\int_0^{\beta\hbar}H(\tau)d\tau\right]=\sum_{b^{(0)},\ldots,b^{(P)}=1}^{N}\prod_{\alpha=0}^{P-1}\langle\bar{b}^{(\alpha)}|e^{-\epsilon\bar{H}^{(\alpha)}}|\bar{b}^{(\alpha+1)}\rangle\prod_{\alpha=0}^{P-1}T^{(\alpha)}_{b^{(\alpha)},b^{(\alpha+1)}}K_{b^{(\alpha+1)}}e^{-\epsilon H^{(\alpha)}_{b^{(\alpha+1)}}}K_{b^{(\alpha+1)}}\ . \tag{8}$$

This is, up to the norming partition function $\bar{Q}(\beta)$ of $\bar{H}$, just the average of the last operator product with respect to the reduced system. The $T_{i,l}$ part represents, of course, just the transitions between different blocks. Such transitions have to follow after every time-slice propagation. Inserting this result in Eq. (3) one furthermore gets for thermal averages

$$Q(\beta)\langle L\rangle_{\text{equ}}=\sum_{b^{(0)},\ldots,b^{(P)}=1}^{N}\prod_{\alpha}\langle\bar{b}^{(\alpha)}\,|\,e^{-\epsilon\bar{H}^{(\alpha)}}\,|\,\bar{b}^{(\alpha+1)}\rangle e^{S_B(L)}\ , \tag{9}$$

where $e^{S_B(L)}$ can be written down explicitly as a trace of a well-defined product of operators. Choosing for L the identity operator we obtain the partition function $Q(\beta)$. We write simply S_B for $S_B(Id)$. The index B reminds us that S_B describes the influence of the block decomposition of H. S_B depends on the specific path $|\bar{b}^{(\alpha)}\rangle$, $\alpha=0,\ldots,P$, through the reduced state space and we denote it sometimes more clearly by $S_B[b^{(\alpha)}]$.

We call S_B the influence phase (of the block decomposition and reduction) of H. That we can write down S_B explicitly enables us to examine a large range of examples; this was never easily done before. The terms "influence functional" and "influence phase" were introduced in the literature some time ago by Feynman and Vernon,[2(b)] and we have to show that our terminology does not contradict theirs. In fact the known terminology is contained in ours, as we now show.

B. Special example

Motivated by the usual reduction of a bath of harmonic oscillators[2(b)] or a bath of two-level systems[4(b)] we treat here as an original system space a tensor product space

$$\mathbb{H}=\hat{\mathbb{H}}\equiv\mathbb{H}_0\otimes\mathbb{H}_1\ , \tag{10}$$

where a time-independent Hamiltonian $\hat{H}$ operates having the form

$$\hat{H}=H_0\otimes Id_{\mathbb{H}_1}+H_I+Id_{\mathbb{H}_0}\otimes H_1 \tag{11}$$

and H_0 and H_1 are defined on $\mathbb{H}_0$ and $\mathbb{H}_1$, respectively. Let $|\sigma\rangle$, $\sigma\in M_0$, an orthonormal basis of $\mathbb{H}_0$ and $|X\rangle$, $X\in M_1$, an orthonormal basis of $\mathbb{H}_1$. Then the dressed states $|\sigma\rangle|X\rangle$ form a basis of the original system space $\hat{\mathbb{H}}$. We consider H_0 as a system Hamiltonian and H_1 as a bath Hamiltonian. The interaction H_I shall be diagonal in the given dressed-state basis. The usual reduction procedure integrates out the dressing of the system states $|\sigma\rangle$. We show that this procedure is equivalent to a reduction in our sense using the following decomposition of $\mathbb{H}$:

$$K_i=\hat{K}_i\equiv|i\rangle\langle i|\otimes Id_{\mathbb{H}_1}\quad\text{for all } i\in M_0\ . \tag{12}$$

Taking now for the reduced space just $\bar{\mathbb{H}}=\mathbb{H}_0$ and for the reduced Hamiltonian $\bar{H}=H_0$ we calculate

$$H_i=K_i(H_I+H_1)K_i$$

and for $i\neq l$

$$T_{i,l}=|i\rangle\langle l|\otimes Id_{\mathbb{H}_1} \tag{13}$$

and get for the influence phase S_B the result

$$S_B[\sigma^{(\alpha)}]=\ln\mathrm{Tr}_{\mathbb{H}_1}e^{-\beta H_1}+\ln\left\langle\exp\left[-\frac{1}{P}\sum_{\alpha=0}^{P-1}\beta c_{\sigma^{(\alpha)},X^{(\alpha)}}\right]\right\rangle_{H_1}\ , \tag{14}$$

where $c_{i,X}\equiv\langle X|\langle i|H_I|i\rangle|X\rangle$ is the coupling matrix element and $\langle\cdots\rangle_{H_1}$ denotes the usual path average with respect to the operator H_1, i.e., for a functional $F[\sigma^{(\alpha)},X^{(\alpha)}]$,

$$\langle F[\sigma^{(\alpha)},X^{(\alpha)}]\rangle_{H_1}\equiv\sum_{\{X^{(\alpha)}\}}\frac{\prod_{\alpha=0}^{P-1}\langle X^{(\alpha)}|e^{-\epsilon H_1}|X^{(\alpha+1)}\rangle}{\mathrm{Tr}e^{-\beta H_1}}\times F[\sigma^{(\alpha)},X^{(\alpha)}]\ . \tag{15}$$

The result is a functional of $\sigma^{(\alpha)}$ alone. Equation (14) is in fact used traditionally, e.g., in deriving the influence phase for a harmonic bath. In the harmonic-bath case the average $\langle\cdots\rangle_{H_1}$ can be done analytically with Gaussian integrals.[6] For brevity we will not repeat the standard procedure to derive the influence phase for a harmonic bath; but we collect the results which we will use in Sec. V and make some clarifying remarks. The dressed-states model is not only a specific example for us; properly extended, the dressed-states model will even contain the general theory mentioned in Sec. II A, and therefore provides just another interpretation for the reduction process.

C. Restatement of the dressed-states model

Let $\mathbb{H}_0$ be a Hilbert space with an orthonormal basis $|\sigma\rangle$, $|\sigma\rangle\in M_0$, and for every $\sigma\in M_0$, let $\mathbb{H}_\sigma$ be a Hilbert space. Now we dress any state $|\sigma\rangle$, $\sigma\in M_0$, with its specific bath $\mathbb{H}_\sigma$ and define the original system space $\hat{\mathbb{H}}$ as the following direct sum:

$$\hat{\mathbb{H}}\equiv\bigoplus_{\sigma\in M_0}[(\mathbb{C}|\sigma\rangle)\otimes\mathbb{H}_\sigma]\ . \tag{16}$$

Now we define a complete set $\hat{K}_i$, $i\in M_0$, of orthogonal projectors on $\hat{\mathbb{H}}$ by

$$\hat{K}_i\equiv|i\rangle\langle i|\otimes Id_{\mathbb{H}_i}\ . \tag{17}$$

One discovers immediately that the example in Sec. II B is just the special case where all the bath spaces $\mathbb{H}_\sigma$ are

the same. On the other hand, there is even an isomorphism between the general theory in Sec. II A and the model here because the direct product notation in Eq. (16) is trivial up to an isomorphism. $(\mathbb{C}|\sigma\rangle)\otimes\mathbb{H}_\sigma$ is of course isomorphic to $\mathbb{H}_\sigma$ and therefore $\hat{\mathbb{H}}$ is isomorphic to the direct sum of $\mathbb{H}_\sigma$,

$$\hat{\mathbb{H}}\simeq\bigoplus_{\sigma\in M_0}\mathbb{H}_\sigma\equiv\mathbb{H}\ . \tag{18}$$

This isomorphism includes operators in the sense that linear operators $\hat{L}$ on $\hat{\mathbb{H}}$ correspond uniquely to operators L on $\mathbb{H}$. First we set K_i equal to the canonical projector of the direct sum $\mathbb{H}$ on $\mathbb{H}_i$. Then we assign

$$L=\sum_{i,l\in M_0}K_iLK_l\mapsto\sum_{i,l\in M_0}|i\rangle\langle l|\otimes\bar{L}_{i,l}\equiv\hat{L}\ , \tag{19}$$

where $\bar{L}_{i,l}$ denotes the operator K_iLK_l restricted to the subspaces $\mathbb{H}_l$ and $\mathbb{H}_i$. There is an interesting interpretation of this mapping. One can imagine that L is a big matrix defined on the space $\mathbb{H}$. The operator sum on the left-hand side of Eq. (19) describes an additive decomposition of L into its subspace components. All the parts K_iLK_l have, as a matrix, the same size as L. $\bar{L}_{i,l}$ are in general smaller matrices, namely, the nontrivial part of K_iLK_l. To know only the submatrices $\bar{L}_{i,l}$ is unfortunately not enough to build up the matrix L because $\bar{L}_{i,l}$ does not specify into which block location (i,l) of L it has to be inserted. But the tensor product $|i\rangle\langle l|\otimes\bar{L}_{i,l}$ contains the full information we need; the operator $|i\rangle\langle l|$ acts as a pointer to the right location within L. Deriving now the influence phase S_B in the space $\hat{\mathbb{H}}$, we end up with the formula

$$S_B[b^{(\alpha)}]=\ln\mathrm{Tr}_{\mathbb{H}_{b^{(0)}}}\left[\prod_{\alpha=0}^{P-1}\bar{T}_{b^{(\alpha)},b^{(\alpha+1)}}e^{-\epsilon\bar{H}_{b^{(\alpha+1)}}}\right]\ , \tag{20}$$

where for equal indices $\bar{T}_{i,i}$ is the identity operator on the space $\mathbb{H}_i$. S_B defined as in Eq. (9) in the time-independent case and the functional S_B here in Eq. (20) are, of course, the same. There is only a slight difference in the organization of the calculation. In Sec. II A we used submatrices of H imbedded properly in matrices of the size of H for the calculation. The transition matrices $T_{i,l}$ described jumps from the i block of a big matrix to the l block *and* the connection of different short-time propagators. In Eq. (20) we work only with the submatrices, denoted by the overbar. The trace with respect to the pointer space $\mathbb{H}_0$ is already carried out. Of course, the isomorphism described here is also valid in the case of a time-dependent Hamiltonian, we just suppressed time-dependency for notational simplicity.

III. TECHNIQUES FOR EVALUATION OF INFLUENCE FUNCTIONALS

A. Permutationlike transitions and separable transitions

Equations (5) and (6) lead to the following representations of the original Hamiltonian H and the reduced Hamiltonian $\bar{H}$:

$$H^{(\alpha)}=\sum_{i=1}^{N}(H_i^{(\alpha)}+\bar{h}_i^{(\alpha)}K_i)+\sum_{\substack{i,l=1\\ i<l}}^{N}(\bar{t}_{i,l}^{(\alpha)}T_{i,l}^{(\alpha)}+\text{adjoint})\ , \tag{21}$$

$$\bar{H}^{(\alpha)}=\sum_{i=1}^{N}\bar{h}_i^{(\alpha)}|\bar{i}\rangle\langle\bar{i}|+\sum_{\substack{i,l=1\\ i<l}}^{N}(\bar{t}_{i,l}^{(\alpha)}|\bar{i}\rangle\langle\bar{l}|+\text{adjoint})\ . \tag{22}$$

We omit the time dependence via α in the following for simplicity. The reduction process of an original system defined above leads, according to Eq. (9), to the reduced Hamiltonian $\bar{H}$ *and* the influence phase S_B describing the influence of the reduction. For further treatment the reduced Hamiltonian has, of course, to be considered as the easy, solvable part whereas the influence phase S_B represents the difficult part characterizing the much more complicated original-system behavior. In this section we show how to produce, in important cases, formulas in closed form for the influence phase S_B by choosing the parameters $\bar{h}_i$ and $\bar{t}_{i,l}$ of the reduced Hamiltonian so that the influence phase S_B will be small compared to the reduced Hamiltonian. The transition operators $T_{i,l}$ play, due to Eq. (8), an important role in the calculation of the influence phase S_B. But these operators also occur in Eq. (21) for the Hamiltonian. Comparison of Eqs. (21) and (22) leads to the conclusion that $\bar{H}$ will describe H better if the transition operators $T_{i,l}$ have more algebraic properties of the operators $|\bar{i}\rangle\langle\bar{l}|$, and then the influence S_B is expected to be less serious. First we observe for the coupling part of the Hamiltonian H

$$(tT_{i,l}^{(\alpha)}\pm t^*T_{i,l}^{(\alpha)\dagger})(tT_{i,l}^{(\alpha+1)}\pm t^*T_{i,l}^{(\alpha+1)\dagger})=\pm|t|^2(T_{i,l}^{(\alpha)}T_{l,i}^{(\alpha+1)}+T_{l,i}^{(\alpha)}T_{i,l}^{(\alpha+1)})\ . \tag{23}$$

The right-hand side of this equation shows that this operator acts on the subspaces $\mathbb{H}_i$ and $\mathbb{H}_l$ alone and we can evaluate functions of this coupling part readily if these operators on $\mathbb{H}_i$ and $\mathbb{H}_l$ are projectors. Motivated by these observations we examine here, in the time-independent case, the following basic property of the transition operators $T_{i,l}$.

Definition. Let $K_i^{(l)}\equiv T_{i,l}T_{l,i}$ and $K_l^{(i)}\equiv T_{l,i}T_{i,l}$. We say that a pair (i,l) leads to a permutation like transition if and only if $K_i^{(l)}$ and $K_l^{(i)}$ are projectors.

We first remark that in the special dressed-states example in Sec. II B *all* the transition operators $T_{i,l}$ are permutationlike and even have maximal rank, $K_i^{(l)}=K_i$ and $K_l^{(i)}=K_l$, there. With the definition of permutationlike transitions we extracted the basic algebraic idea which made the dressed-states model tractable. The most powerful method we can get is a combination of permutationlike transitions of maximal rank as in the special dressed-states model and permutationlike transitions of minimal rank defined below as separable transitions. But before we do so, we justify the terminology permutationlike for the projector property of $K_i^{(l)}$: For any analytic

function f one can show with Eq. (23) if the pair (i,l) leads to a permutationlike transition

$$f(tK_i^{(l)}T_{i,l}+t^*K_l^{(i)}T_{l,i})$$
$$=f(0)(Id-K_i^{(l)}-K_l^{(i)})+f_+(|t|)(K_i^{(l)}+K_l^{(i)})$$
$$+f_-(|t|)\left[\frac{t}{|t|}K_i^{(l)}T_{i,l}+\frac{t^*}{|t|}K_l^{(i)}T_{l,i}\right], \quad (24)$$

where f_+ and f_- represent the even and the odd part of f, respectively. Using this result for the function $f(z)\equiv 1+z-z^2$ one sees immediately that the operator

$$P_{i,l}\equiv f(K_i^{(l)}T_{i,l}+K_l^{(i)}T_{l,i})$$
$$=Id-K_i^{(l)}-K_l^{(i)}+K_i^{(l)}T_{i,l}+K_l^{(i)}T_{l,i} \quad (25)$$

is a permutation of the spaces $K_i^{(l)}(\mathbb{H}_i)$ and $K_l^{(i)}(\mathbb{H}_l)$, i.e., $P_{i,l}$ is unitary and Hermitian and

$$P_{i,l}K_i^{(l)}P_{i,l}=K_l^{(i)} . \quad (26)$$

We will use this property later for expressing exponential operators after a transformation with the permutations $P_{i,l}$ by exponentials of the transformed original operators. If the permutation property is fulfilled the remark after Eq. (20) that the operators $T_{i,l}$ describe jumps from the i block of a big matrix to the l block can be visualized nicely.

Now we give the second basic definition and show how it meets the permutation property.

Definition. We say that a pair (i,l) leads to a separable transition if and only if $T_{i,l}$ is a dyadic product, i.e., $T_{i,l}=\mathbf{w}_{i,l}\mathbf{v}_{i,l}^\dagger$ for states $\mathbf{w}_{i,l}$ and $\mathbf{v}_{i,l}$ in the original system space.

One easily verifies that separable transitions are permutationlike up to a norm factor: With $T_{i,l}=\mathbf{w}_{i,l}\mathbf{v}_{i,l}^\dagger$,

$$(T_{i,l}T_{l,i})^2=|\mathbf{v}_{i,l}|^2|\mathbf{w}_{i,l}|^2T_{i,l}T_{l,i} , \quad (27)$$

and therefore $T_{i,l}$ is permutationlike if the vectors $\mathbf{w}_{i,l}$ and $\mathbf{v}_{i,l}$ are normed to unity. Therefore it will be convenient to choose $\bar{t}_{i,l}$ in this case so that the vectors $\mathbf{v}_{i,l}$ and $\mathbf{w}_{i,l}$ are normed. We also observe from $T_{i,l}^2=0$ that for a nontrivial separable transition the vectors $\mathbf{v}_{i,l}$ and $\mathbf{w}_{i,l}$ are orthogonal to one another. If $T_{i,l}=\mathbf{w}_{i,l}\mathbf{v}_{i,l}^\dagger$ with normed vectors $\mathbf{w}_{i,l}$ and $\mathbf{v}_{i,l}$ then the associated permutation $P_{i,l}$, see Eq. (25), permutes just the orthonormal states $\mathbf{w}_{i,l}$ and $\mathbf{v}_{i,l}$. Further, permutationlike transitions form a closed algebra in the sense that with $T_{i,l}$ and $T_{l,n}$ the product $T_{i,l}T_{l,n}$ is also a dyadic product. Separable transitions can immediately be used to characterize the influence phase S_B for block decompositions for special paths by memory functions. First we observe that for a separable $T_{i,l}$,

$$\mathrm{Tr}(A_1T_{i,l}A_2)=\mathbf{v}_{i,l}^\dagger A_2A_1\mathbf{w}_{i,l} \quad (28)$$

for arbitrary operators A_1 and A_2, i.e., if there is at least one separable transition contained in a path $|\bar{b}^{(\alpha)}\rangle$, $\alpha=0,\ldots,P-1$, then $S_B[b^{(\alpha)}]$ can be expressed by the logarithm of a quadratic form. Therefore we define for pairs (i,l) and (m,n), which lead to separable transitions, a memory function $Y_{i,l;m,n}$,

$$Y_{i,l;m,n}(A)\equiv\ln(\mathbf{v}_{i,l}^\dagger A\mathbf{w}_{m,n})$$
for arbitrary operators A . (29)

Then the right-hand side of Eq. (28) is just $\exp[Y_{i,l;i,l}(A_2A_1)]$. An important case is if all transition operators are separable. Then the functional S_B can be described by memory functions $Y_{i,l;m,n}(A)$, where the operators A are simple propagators in time of the Hamiltonian blocks H_i defined in Eq. (6). In general we observe for separable pairs (i,l), (m,n), and (p,q) the possibility of decomposition for the memory,

$$Y_{i,l;m,n}(A_1T_{p,q}A_2)=Y_{i,l;p,q}(A_1)+Y_{p,q;m,n}(A_2) . \quad (30)$$

One of the most successful tools to write down the influence phase S_B for examples explicitly is to determine the separable transitions and to decompose paths maximally. The reason we call Y a memory will become clearer with the application of the preceding idea, especially if we have developed enough formulas parallel to the harmonic-bath case so that we can compare Y with the well-known memory function for a harmonic bath. While it was very obvious how to use separable transitions after having worked out Eq. (28), we have to think about a more fundamental principle of physics in order to take advantage of the permutation like transitions of maximal rank.

B. Symmetry properties and permutationlike transitions

Nonseparable permutationlike transitions $T_{i,l}$ are most effective to calculate influence phases if their corresponding permutations, Eq. (25), represent symmetries of the given Hamiltonian H, Eq. (21), or of a modified dimensionless sub-Hamiltonian, e.g.,

$$h\equiv\sum_{i\in N_0}\beta H_i+\sum_{\substack{i,l\in N_0\\ i\neq l}}T_{i,l} , \quad (31)$$

where N_0 is a subset of the set $\{0,\ldots,N\}$. One shows straightforwardly that for a permutationlike transition the symmetry property

$$HP_{i,l}=P_{i,l}H \quad (32)$$

is equivalent to the following five equations:

$$\mathrm{Im}(H_iK_i^{(l)})=\mathrm{Im}(\bar{t}_{i,l})K_i^{(l)} , \quad (33a)$$

$$\mathrm{Im}(H_lK_l^{(i)})=-\mathrm{Im}(\bar{t}_{i,l})K_l^{(i)} , \quad (33b)$$

$$(H_l+\bar{h}_lK_l)(T_{l,i}K_i^{(l)})=(T_{l,i}K_i^{(l)})(H_i+\bar{h}_iK_i) , \quad (33c)$$

$$\bar{t}_{m,l}T_{m,l}T_{l,i}K_i^{(l)}=\bar{t}_{m,i}T_{m,i}K_i^{(l)} \text{ for all } m\neq i,l , \quad (33d)$$

$$\bar{t}_{m,i}T_{m,i}T_{i,l}K_l^{(i)}=\bar{t}_{m,l}T_{m,l}K_l^{(i)} \text{ for all } m\neq i,l , \quad (33e)$$

where we used for an arbitrary operator A the abbreviation $\mathrm{Im}(A)\equiv(A-A^\dagger)/(2i)$. Similar conditions can, of course, be written down if h, Eq. (31) or any other modification of H commutes with the permutation $P_{i,l}$.

In that way we obtain a scheme for treating partial symmetries of a Hamiltonian.

Now let us discuss permutationlike transitions of maximal rank, i.e., we assume now $K_i^{(l)}=K_i$ and $K_l^{(i)}=K_l$. Then the first two equations (33a) and (33b) just demand that $\bar{t}_{i,l}$ is real. In the last two equations (33d) and (33e) one can omit the factors $K_i^{(l)}$ and $K_l^{(i)}$. These two equations enable us to contract some sequences of transitions to much shorter sequences. Furthermore, we obtain from these equations for $m\neq i,l$ the relation

$$|\bar{t}_{m,l}|^2 K_m^{(l)}=|\bar{t}_{m,i}|^2 K_m^{(i)} . \tag{34}$$

A very important tool follows from Eq. (33c), namely, that the commutator

$$[H_i, T_{i,l} H_l T_{l,i}]=0 . \tag{35}$$

We could write here $P_{i,l}$ instead of $T_{i,l}$ concluding that the permutation $P_{i,l}$ transforms in some sense H_i into H_l and vice versa. From this we get for the following piece of path occurring in the calculation of the influence phase S_B:

$$(K_i e^{-k_1 \epsilon H_i} K_i) T_{i,l} (K_l e^{-k_2 \epsilon H_l} K_l) = K_i e^{-k_1 \epsilon H_i - k_2 \epsilon T_{i,l} H_l T_{l,i}} T_{i,l} . \tag{36}$$

Equation (36) combined with the memory Y, is the chief instrument to writing influence phases explicitly. Here we make clear that this equation arises from symmetry properties of the Hamiltonian. One easily verifies—starting from Eq. (31) with $\{i,l\}\subseteq N_0$—that partial symmetries are enough to obtain Eq. (36).

Let us discuss briefly what the symmetry properties mean in the special dressed-states example in Sec. II B. We already said that in this example all the transition operators are permutationlike of maximal rank. We calculate for the corresponding permutations

$$P_{i,l}=P_{i,l}^0 \otimes Id_{H_1} , \tag{37a}$$

where $P_{i,l}^0$ is an *ordinary* permutation matrix in the space $\mathbb{H}_0$,

$$P_{i,l}^0=Id_{\mathbb{H}_0}-|i\rangle\langle i|-|l\rangle\langle l|+|i\rangle\langle l|+|l\rangle\langle i| . \tag{37b}$$

We then interpret the operators $|i\rangle\langle l|$ as pointers to a certain block location, visualizing the effect of $P_{i,l}$ as a proper permutation of two blocks. Equations (33a), (33b), (33d), and (33e) are fulfilled for the modified Hamiltonian h, Eq. (31), with N_0 the whole set $\{0,\ldots,N\}$. Equation (33c) is in general not true, it is equivalent to the condition that the i and l block of the interaction are equal, i.e., $\langle i|H_I|i\rangle=\langle l|H_I|l\rangle$.

C. Eigenvector part of influence phases

Whereas we have discussed until now algebraic properties of transitions, we consider here, in contrast, paths where no knowledge about transitions is required: the paths without transitions or constant paths. For a path $b^{(\alpha)}$, which is i for all values of α, one gets immediately

$$S_B[b^{(\alpha)}\equiv i]=\ln(\mathrm{Tr} K_i e^{-\beta H_i} K_i)\equiv \ln(\mathrm{Tr}_i e^{-\beta H_i}) , \tag{38}$$

the free energy of a system described by the Hamiltonian H_i. If $|\bar{i}\rangle$ were an eigenvector of the reduced Hamiltonian $\bar{H}$ then the constant path $b^{(\alpha)}\equiv i$ would be the only one containing i for some time α and delivering a finite Boltzmann weight. Eigenvectors are time invariant. In general, we declare the eigenvector part S_{EV} of the influence phase S_B as

$$S_{\mathrm{EV}}[b^{(\alpha)}]\equiv \sum_{i=1}^{N} \ln(\mathrm{Tr}_i e^{-\beta H_i}) \prod_{\alpha=0}^{P} \bar{n}_i^{(\alpha)} . \tag{39}$$

S_{EV} checks the contributions of S_B if the system stays all the time in one and the same subspace $\mathbb{H}_i$. $\bar{n}_i^{(\alpha)}=0,1$ is the occupation number of the reduced state $|\bar{i}\rangle$ at imaginary time α. It checks the occupation of the space $\mathbb{H}_i$ at time α. For nonconstant paths $b^{(\alpha)}$, $S_{\mathrm{EV}}[b^{(\alpha)}]=0$; for finite N especially the handling of S_{EV} requires a finite number of operations and therefore S_{EV} is a solvable part of the influence phase, exactly as the matrix problem $\bar{H}$ is considered to be solvable. For any specific model of H and reduction, the eigenvector part S_{EV} is with certainty a part of the influence phase S_B. We define the rest of S_B, namely, the complicated part,

$$S_B^0\equiv S_B-S_{\mathrm{EV}} . \tag{40}$$

The superscript 0 reminds us that this part of S_B vanishes for constant paths. The decomposition of S_B into an eigenvector part and a remainder (in general complicated) will play a fundamental role for variational calculations. S_{EV} creates, for every reduced state, a reference line, the free energy of the Hamiltonian H_i, around which the real system fluctuates. One expects very good results if one adjusts variationally a parametrized Hamiltonian $\bar{H}$ and an influence phase S_{EV} neglecting S_B^0. Having in mind a trick that martingale theory is based upon, one could extend the decomposition of S_B also, treating paths separately which are constant from time 0 to $\beta\hbar/2$ and from $\beta\hbar/2$ to $\beta\hbar$ but have a transition at time $\beta\hbar/2$ and so on. A distribution can be characterized not only by its moments but also by partial averages. However, we restrict ourselves to the first step, the "mean spherical approximation" only pulling out S_{EV}, and not considering further paths with a finite number of kinks.

If $S_B^0\equiv 0$ we can show an obvious physical interpretation for the eigenvector part S_{EV} because in that case S_{EV} is just the influence phase S_B for block decomposition of H. In fact we can show that there exits in any case a Hamiltonian H' which delivers, after reduction to $\bar{H}$, just S_{EV} as influence phase of the reduction. With a Hamiltonian, a physical interpretation of S_{EV} is constructed. Note that the eigenvector part S_{EV} competes with the diagonal of $\bar{H}$, i.e., with the levels of the reduced system, as one can see from the values of the total action functional S for constant paths,

$$S[b^{(\alpha)}\equiv i]=\ln(e^{-\beta\bar{h}_i}\mathrm{Tr}_i e^{-\beta H_i})=\ln(\mathrm{Tr}_i e^{-\beta K_i H K_i}) . \tag{41}$$

In order to separate the two components we extend $\bar{H}$ to H'. Let

$$a_i \equiv -\frac{1}{\beta}\ln(\mathrm{Tr}_i e^{-\beta H_i}-1) \quad \text{for } i=1,\ldots,N \tag{42}$$

and define a $(2N)\times(2N)$ matrix H' by putting $\bar{H}$ in the left corner and making the rest diagonal with $\bar{h}_i+a_i$ in the $(N+i)$th diagonal place. Identifying now via a projector K_i' level i and level $N+i$, one can easily see that the reduction of H' to $\bar{H}$ delivers just S_{EV} as the influence of the reduction. The construction of H' is not unique. Of course, one can use a larger diagonal part and then identify more levels. Once again, the name "eigenvector part" for S_{EV} is justified by the form of H'. We remark that $\mathrm{Tr}_i e^{-\beta H_i}$ might be smaller than 1 and therefore a_i is not necessarily real and H' can be a complex Hamiltonian. The preceding interpretation of $\bar{H}$ together with S_{EV} can naturally lead not only to shifted energy levels but also to certain lifetimes. H might already be H'. We then obtain from the above certain cases where the eigenvalue problem of H is exactly solvable by a matrix problem. Embedding $\bar{H}$ in the larger H' does *not* mean that we go back to our old "large" Hamiltonian H. The second N lines of H' are diagonal and therefore trivial. It just shows in a compact way that the problem with $S_B \equiv S_{\mathrm{EV}}$ is solved if $\bar{H}$ is diagonalized. But this reflects just the fact that only N constant paths are necessary to describe S_{EV} completely.

IV. CHARACTERISTIC EXAMPLES

The discussion up to this point has been rather formal, stressing the separation of the influence functional into an eigenvalue part and a (more complicated) remainder, as well as the nature of the various types of transition. It seems appropriate to give some simple examples in which this sort of analysis is applied to reasonable model problems.

A. Discretized Laplacian with cyclic closure modulo 4

We study here the 4×4 Hamiltonian matrix

$$H=\begin{bmatrix} 2E_0 & \Delta & 0 & \Delta \\ \Delta & 2E_0 & \Delta & 0 \\ 0 & \Delta & 2E_0 & \Delta \\ \Delta & 0 & \Delta & 2E_0 \end{bmatrix} \tag{43}$$

using the partitioning

$$\begin{aligned} K_1 &= |1\rangle\langle 1| + |2\rangle\langle 2| \ , \\ K_2 &= |3\rangle\langle 3| + |4\rangle\langle 4| \ , \end{aligned} \tag{44}$$

and the reduced Hamiltonian

$$\bar{H}=\begin{bmatrix} 2E_0 & \Delta \\ \Delta & 2E_0 \end{bmatrix} , \tag{45}$$

where $|1\rangle,\ldots,|4\rangle$ is the canonical basis of $\mathbb{R}^4$ and E_0 and Δ are real parameters.

There are several realizations of this Hamiltonian. First H is the topological matrix of a Hückel treatment of cyclobutadiene. Reduction with K_1 and K_2 identifies carbon atoms so that the cyclobutadiene is contracted to an ethylene molecule. Second, H is the Hamiltonian for the simplest singlet–molecular-orbital treatment of the hydrogen molecule H_2 assuming a $1s$ orbital with α and β spin localized at every H atom as the fundamental atomic orbitals. The two spin wave functions $|1\rangle$ and $|3\rangle$ represent neutral structures whereas $|2\rangle$ and $|4\rangle$ represent ionic ones. Third, we remark that the double-symmetric difference ∇^2,

$$\nabla^2 a_l \equiv a_{l+1}-2a_l+a_{l-1} \ , \tag{46}$$

for any sequence a_l, $l\in\mathbb{N}$, has, modulo 4 with cyclic closure, H as matrix representation with $\Delta=1$, $E_0=-1$. In other words, H describes a discretized free particle problem with cyclic closure.

Of course, the eigenvalue problem of H can be solved immediately but here we want to demonstrate how the reduction technique works and how the influence phase S_B is obtained. We have a simple situation where all transitions are (not trivial but) permutationlike of maximal rank. The parts H_1, H_2 and $T_{1,2}$ of H, Eq. (6), are all equivalent to the 2×2 permutation matrix $|1\rangle\langle 2|+|2\rangle\langle 1|$,

$$\begin{aligned} H_1 &= \Delta[\,|1\rangle\langle 2| + |2\rangle\langle 1|\,] \ , \\ H_2 &= \Delta[\,|3\rangle\langle 4| + |4\rangle\langle 3|\,] \ , \\ T_{1,2} &= |1\rangle\langle 4| + |2\rangle\langle 3| \ . \end{aligned}$$

Therefore we find that $T_{1,2}$ is permutationlike with

$$K_1^{(2)} \equiv T_{1,2}T_{2,1}=K_1, \quad K_2^{(1)} \equiv T_{2,1}T_{1,2}=K_2 \ ,$$

and further that the permutation $P_{1,2}=T_{1,2}+T_{2,1}$ just permutes H_1 and H_2,

$$H_2 = T_{2,1}H_1T_{1,2} \ , \tag{47}$$

i.e., we can apply Eq. (36) to evaluate the influence functional and discover that it is independent of time, even independent of the selected path,

$$S_B[b^{(\alpha)}]=S_B(\beta):=\ln \mathrm{Tr}_1 e^{-\beta H_1}=\ln[2\cosh(\beta\Delta)] \ . \tag{48}$$

Actually, the permutation $P_{1,2}$ permutes even with the Hamiltonian H, i.e., Eq. (32) is true and the time invariance of S_B is a consequence of symmetries. Because of this time invariance the partition function $Q(\beta)$ of H is the partition function of $\bar{H}$ up to the factor e^{S_B}. Furthermore, the equilibrium average of the energy is the same for the original and the reduced system,

$$Q(\beta)=e^{S_B(\beta)}\mathrm{Tr}e^{-\beta\bar{H}}=(e^{-\beta(E_0+\Delta)}+e^{-\beta(E_0-\Delta)})^2 \ . \tag{49}$$

The reduction formalism enables us to use symmetries immediately for the calculation of partition functions without doing a spectral decomposition first. Of course, we can give the square form of the partition function $Q(\beta)$, Eq. (49), by just interpreting H as the molecular orbital (MO) Hamiltonian of H_2. In this case, no calculation needs to be done because in the MO picture the two electrons of H_2 are treated as noninteracting particles, if

Coulomb repulsions are ignored.

We remark that one might also think of identifying, in the H_2 case, the homopolar structures on one hand and the ionic ones on the other hand. This procedure would correspond to a new partitioning marked by primes,

$$K_1' = |1\rangle\langle 1| + |3\rangle\langle 3| ,$$
$$K_2' = |2\rangle\langle 2| + |4\rangle\langle 4| , \tag{50}$$
$$\bar{H}' = 2\begin{bmatrix} E_0 & \Delta \\ \Delta & E_0 \end{bmatrix} .$$

Then one gets $H_1' = H_2' \equiv 0$ and the transition $T_{1,2}'$ is separable and permutationlike,

$$T_{1,2}' = (K_1'\mathbf{v})^0 (K_2'\mathbf{v})^{0\dagger} , \tag{51}$$

where $\langle i | \mathbf{v} = 1$ for all $i = 1, \ldots, 4$. In this case the influence phase S_B' is totally defined by the transitions. One can easily show that then S_B' is equal to its eigenvector part and

$$S_B' = S_{\mathrm{EV}}' = \ln(2)\left[\prod_{\alpha=0}^{P-1} \bar{n}_1^{(\alpha)} + \prod_{\alpha=0}^{P-1} \bar{n}_2^{(\alpha)}\right] . \tag{52}$$

Here is $K_1^{(2)\prime} \neq K_1'$ and $K_2^{(1)\prime} \neq K_2'$, but nevertheless the permutation $P_{1,2}'$ commutes with H, as one can see from Eqs. (33). Thus the primed decomposition is a decomposition by symmetries but less trivial then our original decomposition.

B. One-fermion problem

In our next example we use memory functions rather than symmetries. But for demonstration we restrict it again to a simple case. In Ref. 4(a) the one-fermion hole system was reduced to a two-state system. Of course, fermions and fermion holes are isomorphic. We reformulate here the simplest case, namely, the reduction of three one-fermion states which are occupied by one fermion to a two-state system. We study the 3×3 Hamiltonian matrix

$$H = \begin{bmatrix} \eta_1 & t_{1,2} & t_{1,3} \\ t_{1,2}^* & \eta_2 & t_{2,3} \\ t_{1,3}^* & t_{2,3}^* & \eta_3 \end{bmatrix} \tag{53}$$

using the partitioning

$$K_1 = |1\rangle\langle 1| ,$$
$$K_2 = |2\rangle\langle 2| + |3\rangle\langle 3| , \tag{54}$$

and a two-level system as the reduced Hamiltonian $\bar{H}$

$$\bar{H} = \begin{bmatrix} \eta_1 & -z \\ -z^* & h_2 \end{bmatrix} , \tag{55}$$

where $|1\rangle$, $|2\rangle$, and $|3\rangle$ denote the canonical basis of $\mathbb{C}^3$. η_i and h_2 are real parameters, and $t_{i,l}$ and z complex parameters.

First we discuss a realization of the Hamiltonian, Eq. (53). For one available fermion H is isomorphic to the Hamiltonian H',

$$H' \equiv \sum_{i=1}^{3} \eta_i a_i^\dagger a_i + \sum_{1\le i<l\le 3} (t_{i,l} a_i^\dagger a_l + \text{adjoint}) , \tag{56}$$

where a_i are annihilation operators for fermions and the adjoint $a_i^\dagger$ the corresponding creation operators. Using the Hamiltonian H, Eq. (53), we intend to integrate out two secondary one-electron levels η_2 and η_3 and to keep one primary level η_1 untouched. The three states $|1\rangle$, $|2\rangle$, and $|3\rangle$ can be characterized by their occupation numbers $m_i = 0, 1$, which determine the occupation of state i with the fermion. $|i\rangle$ is the "determinant" wave function

$$|i\rangle = |m_1 m_2 m_3\rangle \tag{57}$$

with $m_i = 1, m_l = 0$ for $l \neq i$. The occupation numbers m_i are here not only one-fermion level occupation numbers but also occupation numbers for the real states $|i\rangle$. Since we have only one fermion available this statement is of course trivial.

Now we determine the influence phase S_B. We write here S_{sec} for S_B to indicate that we contracted the two secondary states. Equation (39) gives immediately the eigenvector part S_{EV} of S_{sec},

$$S_{\mathrm{EV}} = \ln(\mathrm{Tr}_{\mathrm{sec}} e^{-\beta H_2}) \prod_{\alpha=0}^{P-1} (1 - m_1^{(\alpha)}) , \tag{58}$$

where H_2 is defined in Eq. (6), $\mathrm{Tr}_{\mathrm{sec}}$ is an abbreviation for $\mathrm{Tr}(K_2 \cdots K_2)$, and $m_1^{(\alpha)} = 0, 1$ is the occupation of the primary level η_1 at imaginary time α. The rest $S_{\mathrm{sec}}^0 \equiv S_B^0$ of S_B depends on the transitions. But there exists only one transition matrix $T_{i,l} = T_{1,2}$ and this matrix is separable,

$$T_{1,2} = -K_1 H K_2 / z = -|1\rangle \frac{\langle 1 | H K_2}{z} . \tag{59}$$

Taking for z the norm $(|t_{1,2}|^2 + |t_{1,3}|^2)^{1/2}$ of the transition vector $\langle 1 | H K_2 \neq 0$ we get $T_{1,2}$ to be permutationlike. In general S_{sec}^0 can be expressed by a memory function defined in Eq. (29),

$$Y(\tau) \equiv Y_{1,2;2,1}(K_2 e^{-\tau\beta H_2} K_2)$$
$$= \ln[\langle 1 | H K_2 e^{-\tau\beta H_2} (H K_2)^\dagger | 1\rangle / |z|^2] , \tag{60}$$

with $0 \le \tau \le 1$. Proper decompositions of paths in the reduced two-level space shows that

$$S_{\mathrm{sec}} = \sum_{k=0}^{P-1} \sum_{\alpha=0}^{P-1} Y\left[\frac{k}{P}\right] m_1^{(\alpha)} \prod_{\gamma=1}^{k+1} (1 - m_1^{(\alpha+\gamma)}) m_1^{(\alpha+k+2)} . \tag{61}$$

The product over occupation numbers describes quite clearly what we mean by proper decomposition of paths. Not the memory function alone but the function Y *together* with the product of occupation numbers (long range in time) has to be considered as the memory of the reduction process. The difference to the well-known memory of a harmonic bath is first structural: the product over γ would not be there in the harmonic-bath case. Second, the form of the memory function, Eq. (60), is

different in the harmonic-bath case. But there are also similarities, namely, the rest of the structure of Eq. (61). We will discuss this point later.

Besides imaginary time the influence phase S_B is characterized only by the occupation number m. From this, one might get the impression that we integrated out the two levels η_2 and η_3. In fact one can show by transfer-matrix method that

$$e^{\bar{S}+S_B}=\sum\prod_{\alpha=0}^{P-1}\langle m_1^{(\alpha)}m_2^{(\alpha)}m_3^{(\alpha)}|e^{-\epsilon H}|m_1^{(\alpha+1)}m_2^{(\alpha+1)}m_3^{(\alpha+1)}\rangle\ , \tag{62}$$

where $\bar{S}$ denotes the action functional for the two-level system given by $\bar{H}$ and the sum extends over all $m_2^{(\alpha)}$, $m_3^{(\alpha)}=0,1$ under the restriction of conservation of particles, i.e., $m_1^{(\alpha)}+m_2^{(\alpha)}+m_3^{(\alpha)}=1$. The transfer matrices we mentioned above are, of course, isomorphic to the matrices H_1, H_2, and $T_{1,2}$. Equation (62) demonstrates an isomorphic way to calculate S_B, a realization of the isomorphism discussed in Sec. II C.

In Sec. VI we will treat an important generalization of this example variationally. But in our special case with H_2 belonging to a two-level system our advantage is that we can write out the memory function Y. We will do so to demonstrate that our general theory only looks simple because it is formulated in a compact way with the basic ideas given in some algebraic definitions. In fact, the general formalism is far from being trivial. Because H_2 is a 2×2 matrix its propagator (and any other function) can be obtained readily by spectral decomposition of H_2: define with the eigenvalues λ_1 and λ_2 of H_2,

$$H_2=\lambda_1 A_1+\lambda_2 A_2\ , \tag{63}$$

the spectral decomposition of H_2. Then the projectors A_1 and A_2 are expressed by the unit matrix Id and H_2 by inserting $A_2=Id-A_1$ leading for any analytic function f in the nontrivial case[9] $\lambda_1\neq\lambda_2$,

$$f(H_2)=\left[\mathrm{Tr}f(H_2)-\frac{\lambda_1 f(\lambda_1)-\lambda_2 f(\lambda_2)}{\lambda_1-\lambda_2}\right]Id+\frac{f(\lambda_1)-f(\lambda_2)}{\lambda_1-\lambda_2}H_2\ . \tag{64}$$

This formula allows us to write down the memory function Y in the form

$$Y(\tau)=\ln\left[\mathrm{Tr}e^{-\tau\beta H_2}-\frac{\lambda_1 e^{-\tau\beta\lambda_1}-\lambda_2 e^{-\tau\beta\lambda_2}}{\lambda_1-\lambda_2}+\frac{e^{-\tau\beta\lambda_1}-e^{-\tau\beta\lambda_2}}{\lambda_1-\lambda_2}(t_{1,2},t_{1,3})^0 H_2\begin{pmatrix}t_{1,2}^*\\ t_{1,3}^*\end{pmatrix}^0\right]\ . \tag{65}$$

Here the $(\cdots)^0$ notation indicates that the vector is normed to unity, and assuming for z the norm of the vector $(t_{1,2},t_{1,3})$. Further, we choose h_2 so that $\mathrm{Tr}H_2=0$, i.e., $h_2=(\eta_2+\eta_3)/2$. Then the secondary part H_2 has the eigenvalues

$$\lambda_{1,2}=\pm\frac{\lambda_1-\lambda_2}{2}=\pm\left[\left(\frac{\eta_2-\eta_3}{2}\right)^2+|t_{2,3}|^2\right]^{1/2}\ . \tag{66}$$

But there is no reason to expect that in Eq. (65) under the logarithm one might find irrational expressions like square roots. In fact, expanding the exponential functions in Eq. (65) leads to the following formulas, valid even for $\lambda_1+\lambda_2\neq0$:

$$\lambda_1^k+\lambda_2^k=2\sum_{\nu=0}^{[k/2]}\begin{bmatrix}k\\2\nu\end{bmatrix}\left(\frac{\lambda_1+\lambda_2}{2}\right)^{k-2\nu}\left(\frac{\lambda_1-\lambda_2}{2}\right)^{2\nu},$$
$$\frac{\lambda_1^k-\lambda_2^k}{\lambda_1-\lambda_2}=\sum_{\nu=0}^{[(k-1)/2]}\begin{bmatrix}k\\2\nu+1\end{bmatrix}\left(\frac{\lambda_1+\lambda_2}{2}\right)^{k-2\nu-1}\times\left(\frac{\lambda_1-\lambda_2}{2}\right)^{2\nu}. \tag{67}$$

The right-hand sides are of course rational in η_2, η_3, and $t_{2,3}$. In Eqs. (67) we developed the basic sum formulas to be used for summing out the occupation numbers m_2 and m_3. The existence and use of the sum formulas Eq. (67) teaches us that our formalism to sum up a subset of paths is not trivial. Furthermore, Eq. (65) tells us something about the nature of the paths summed up,

$$(t_{1,2},t_{1,3})H_2\begin{pmatrix}t_{1,2}^*\\ t_{1,3}^*\end{pmatrix}=(\eta_2-h_2)|t_{1,2}|^2+(\eta_3-h_2)|t_{1,3}|^2+2\,\mathrm{Re}(t_{1,2}t_{2,3}t_{3,1})\ . \tag{68}$$

The only term which is not symmetric in the transitions is the last one. Following in time the two fermion holes instead of the one fermion, one sees that due to this last term the two fermion holes have exchanged their states from time 0 to the end. There are just two different initial (and final) occupations of the holes leading to a complete determination of the system and so leading to the factor 2 in Eq. (68). This does not reflect any antisymmetry of fermion holes, it only reflects the fact that fermion holes are indistinguishable.

C. Four states and two fermions

For the last example of this section we have to combine the two methods demonstrated above. One part of the Hamiltonian can be treated by symmetry, the rest by separable transitions. We start with a physical form for the Hamiltonian, namely, the analog of Eq. (56) but with four orthonormal states instead of three. We insert two fermions so that all the six real states, two fermion states, are given by determinants $|m_1m_2m_3m_4\rangle$ with $m_i=0,1$, the occupation number of single fermion state $a_i^\dagger|0\rangle$, and $m_1+m_2+m_3+m_4=2$. Ordering the basis of two fermion states by

$$
\begin{aligned}
&|1\rangle \equiv |1100\rangle ,\\
&|2\rangle \equiv |0011\rangle ,\\
&|3\rangle \equiv |1010\rangle ,\\
&|4\rangle \equiv |1001\rangle ,\\
&|5\rangle \equiv |0110\rangle ,\\
&|6\rangle \equiv |0101\rangle .
\end{aligned}
\tag{69}
$$

We obtain the following matrix representation of H:

$$
H=\left[\begin{array}{cc|cc|cc}
\eta_1+\eta_2 & 0 & t^*_{2,3} & t^*_{2,4} & -t^*_{1,3} & -t^*_{1,4} \\
0 & \eta_3+\eta_4 & -t_{1,4} & t_{1,3} & -t_{2,4} & t_{2,3} \\
\hline
t_{2,3} & -t^*_{1,4} & \eta_1+\eta_3 & t^*_{3,4} & t^*_{1,2} & 0 \\
t_{2,4} & t^*_{1,3} & t_{3,4} & \eta_1+\eta_4 & 0 & t^*_{1,2} \\
\hline
-t_{1,3} & -t^*_{2,4} & t_{1,2} & 0 & \eta_2+\eta_3 & t^*_{3,4} \\
-t_{1,4} & t^*_{2,3} & 0 & t_{1,2} & t_{3,4} & \eta_2+\eta_4
\end{array}\right] .
\tag{70}
$$

By reduction we want to identify the two states with $m_1=1$ and $m_2=0$ and the two states with $m_1=0$ and $m_2=1$. Then we can characterize the system by the occupation numbers m_1 and m_2 alone. We therefore define four projectors $K_1,\ldots,K_4$ by

$$
\begin{aligned}
&K_1 \equiv |1\rangle\langle 1| ,\\
&K_2 \equiv |2\rangle\langle 2| ,\\
&K_3 \equiv |3\rangle\langle 3| + |4\rangle\langle 4| ,\\
&K_4 \equiv |5\rangle\langle 5| + |6\rangle\langle 6| .
\end{aligned}
\tag{71}
$$

This decomposition of the Hamiltonian H is already indicated in the preceding matrix representation. Denoting the transition vectors by

$$
\begin{aligned}
&\mathbf{s}_{1,1}\equiv(t^*_{2,3},t^*_{2,4}),\quad \mathbf{s}_{1,0}\equiv-(t^*_{1,3},t^*_{1,4}) ,\\
&\mathbf{s}_{0,1}\equiv(-t_{1,4},t_{1,3}),\quad \mathbf{s}_{0,0}\equiv(-t_{2,4},t_{2,3}) ,
\end{aligned}
\tag{72}
$$

we define the reduced Hamiltonian $\overline{H}$ by

$$
\overline{H}\equiv\left[\begin{array}{cccc}
\eta_1+\eta_2 & 0 & |\mathbf{s}_{1,1}| & |\mathbf{s}_{1,0}| \\
0 & \eta_3+\eta_4 & |\mathbf{s}_{0,1}| & |\mathbf{s}_{0,0}| \\
|\mathbf{s}_{1,1}| & |\mathbf{s}_{0,1}| & \eta_1 & t^*_{1,2} \\
|\mathbf{s}_{1,0}| & |\mathbf{s}_{0,0}| & t_{1,2} & \eta_2
\end{array}\right] .
\tag{73}
$$

The transition from state $|1\rangle$ to state $|2\rangle$ is forbidden and therefore the transition matrix $T_{1,2}$ can be chosen arbitrarily. This is caused by the fact that in one time step only one fermion can be moved because H contains no operators $a_i^\dagger a_k^\dagger a_l a_m$. All the other transitions are permutationlike, $T_{3,4}$ even of maximal rank,

$$
T_{3,4}=|3\rangle\langle 5|+|4\rangle\langle 6| .
\tag{74}
$$

By the corresponding permutation just H_3 and H_4 are permuted and Eqs. (35) and (36) can be applied for $i=3$, $l=4$. The consequence is that propagation in the K_3 space and in the K_4 space have the same effect in the influence phase S_B. The effect of transitions from state $|1\rangle$ and $|2\rangle$ to the K_3 and K_4 spaces and back still remains to be studied. The remaining transition matrices are, however, separable (and permutationlike). They are isomorphic to the normed transition vectors. For $i\in\{1,2\}$ and $l\in\{3,4\}$

$$
T_{i,l}\equiv T_{2-m_1,4-m_1'}\cong \mathbf{s}^0_{m_1,m_1'} .
\tag{75}
$$

The indices of the transition vectors characterize the transitions by the occupation numbers m_i. With the occupation numbers $\bar{n}_i$ defined after Eq. (39) one observes the relations

$$
\begin{aligned}
&\bar{n}_1=m_1m_2 ,\\
&\bar{n}_2=(1-m_1)(1-m_2) ,\\
&\bar{n}_3=m_1(1-m_2) ,\\
&\bar{n}_4=(1-m_1)m_2 .
\end{aligned}
\tag{76}
$$

This shows that after reduction the knowledge of the two (primary) occupation numbers m_1 and m_2 is sufficient. Furthermore,

$$
\bar{n}_3+\bar{n}_4=|m_1-m_2| .
\tag{77}
$$

Now all we need to do in order to get a closed formula for the influence phase S_B is to put together the preceding parts of information. We make the following arrangement for the 16 needed memory functions,

$$
Y_{m_1,m_1',m_1'',m_1'''}(\tau)\equiv\ln\left\{\mathbf{s}^0_{m_1,m_1'}\exp\left[-\tau\beta\begin{pmatrix}\eta_3 & t^*_{3,4}\\ t_{3,4} & \eta_4\end{pmatrix}\right]\mathbf{s}^{0+}_{m_1''',m_1''}\right\} ,
\tag{78}
$$

where m_1, m_1', m_1'', and m_1''' are 0 or 1 and $0\le\tau\le 1$. Then we get for $S_B=S_{\mathrm{EV}}+S_B^0$ the following result:

$$
S_{\mathrm{EV}}=\ln\left\{\mathrm{Tr}\exp\left[-\beta\begin{pmatrix}\eta_3 & t^*_{3,4}\\ t_{3,4} & \eta_4\end{pmatrix}\right]\right\}\prod_{\alpha=0}^{P-1}|m_1^{(\alpha)}-m_2^{(\alpha)}| ,
\tag{79}
$$

$$
\begin{aligned}
S_B^0=\prod_{k=0}^{P-2}\sum_{\alpha=0}^{P-1}Y_{m_1^{(\alpha)},m_1^{(\alpha+1)},m_1^{(\alpha+k+1)},m_1^{(\alpha+k+2)}}\left[\frac{k}{P}\right](1-|m_1^{(\alpha)}-m_2^{(\alpha)}|)\\
\times\prod_{\gamma=1}^{k+1}|m_1^{(\alpha+\gamma)}-m_2^{(\alpha+\gamma)}|(1-|m_1^{(\alpha+k+2)}-m_2^{(\alpha+k+2)}|) .
\end{aligned}
\tag{80}
$$

There is a close analogy of this remarkable result to the result of example in Sec. IV B, Eqs. (58) and (61). It becomes apparent that the occupation difference in the two primary levels has here the same effect as the occupation number had in example *B*. Of course, exactly as in the one-fermion example, we can write down the memory functions explicitly. Furthermore, we can show that S_B meets well our starting point in the sense that $\bar{S}+S_B$ can be obtained by integrating out the occupation numbers m_3 and m_4 under conservation of particles, i.e., $\sum_{i=1}^{4} m_i^{(\alpha)}=2$; it is just analogous to Eq. (62).

V. BLOCK DECOMPOSITION AND LINEARLY COUPLED HARMONIC BATHS

A. Theory

We extend here the idea of reducing a harmonic bath to the case where the harmonic bath is coupled linearly to certain projectors instead of simple states and also where the subspaces in which the projectors operate are contracted due to our general theory. To be specific we define an original system space $\mathbb{H}_0$ with a partitioning $\{K_i \mid i=1,\ldots,N\}$ by N orthonormal projectors K_i and a harmonic bath space $\mathbb{H}_1$ as the J-fold ($J\in\mathbb{N}$) tensor product of the space of real functions. A basis of the functions over $\mathbb{R}$ is given by the vectors $|X_j\rangle$, $X_j\in\mathbb{R}$, so that the scalar product $\langle X_j' \mid X_j\rangle$ is just the δ function in X_j-X_j'. The total original space is then spanned by the dressed states $|\sigma\rangle|X_1\rangle\cdots|X_J\rangle$ with $|\sigma\rangle$ in $\mathbb{H}_0$. Now we consider an arbitrary system Hamiltonian H_0 on $\mathbb{H}_0$ coupled linearly by an interaction H_I to a Hamiltonian H_{HB} on $\mathbb{H}_1$, which represents a harmonic bath so that we get a total Hamiltonian H in the form

$$H=H_0+H_I+H_{\mathrm{HB}} \ . \tag{81}$$

By linear coupling in the coordinate we mean

$$H_I(\{X\})=\sum_{j=1}^{J}\sum_{i=1}^{N} K_i c_{i,j} X_j, \quad c_{ij}\in\mathbb{R} \ . \tag{82}$$

The harmonic bath part is as usual

$$H_{\mathrm{HB}}(\{P,X\})=\tfrac{1}{2}\sum_{j=1}^{J}(P_j^2/M_j+M_j\omega_j^2X_j^2) \ , \tag{83a}$$

with mass M_j and frequency ω_j of the jth oscillator and either

$$P_j=P_j^{\mathrm{cl}}=M_j\dot{X}_j \tag{83b}$$

in the case of classical harmonic oscillators or

$$P_j=P_j^{\mathrm{qu}}=-i\hbar\,\partial/\partial X_j \tag{83c}$$

in the case of quantized harmonic oscillators. From time to time we also use the notations $H_{\mathrm{HB}}^{\mathrm{cl}}$ and $H_{\mathrm{HB}}^{\mathrm{qu}}$ to be more specific. The essential difference in the classical and quantum case is that P_j^{cl} commutes with all other parts of H whereas P_j^{qu} does not.

The aim of our reduction is to contract H to a reduced system Hamiltonian $\bar{H}_N$ defined according to Eq. (22) in the time-independent case on the reduced system space $\mathbb{C}^N$. During this procedure we should integrate out the harmonic bath totally. Therefore we use as the reducing projectors on the total original space just $K_i\otimes Id_{\mathbb{H}_1}$ for $i=1,\ldots,N$. Then we obtain for the parts of the Hamiltonian H, Eq. (6), which we need to build up the influence phase S_B,

$$H_i=K_i(H_0)_iK_i+\left[\sum_j c_{i,j}X_j\right]K_i+H_{\mathrm{HB}} \ , \tag{84a}$$

$$T_{i,l}=(T_0)_{i,l}\equiv K_iH_0K_l/\bar{t}_{i,l} \ . \tag{84b}$$

The short-time propagator of H_i restricted to the K_i space can now be factorized into one part originating from the coupling and harmonic bath and a matrix part arising from H_0,

$$K_ie^{-\epsilon H_i}K_i=\exp\left[-\epsilon\left[\sum_j c_{i,j}X_j+H_{\mathrm{HB}}\right]\right]\times K_ie^{-\epsilon K_i(H_0)_iK_i}K_i \ . \tag{85}$$

This results in the fundamental fact that the influence phase S_B is only a sum of the influence phases $(S_0)_B$ for block decomposition of H_0 and the well-known influence phase S_{HB} describing only the reduction of a harmonic bath. Equation (9) now delivers, e.g., for the partition function $Q(\beta)$ of the problem in the quantum-mechanical case,

$$Q(\beta)=\sum e^{(S_0)_B}\int_{-\infty}^{\infty}d\{X^{(0)}\}\cdots\int_{-\infty}^{\infty}d\{X^{(P-1)}\}\langle\{X^{(\alpha)}\}\mid\langle\bar{b}^{(\alpha)}\mid e^{-\epsilon\bar{H}}\mid\bar{b}^{(\alpha+1)}\rangle\mid\{X^{(\alpha+1)}\}\rangle \ . \tag{86}$$

Here the sum runs over all $b^{(0)},\ldots,b^{(P)}$ from 1 to N under cyclic closure $b^{(P)}=b^{(0)}$, and the Hamiltonian $\bar{H}$ is obtained from the total Hamiltonian H, Eq. (81) replacing H_0 by its reduced $\bar{H}_N$ and by replacing in the interaction H_I the projectors K_i by $|\bar{i}\rangle\langle\bar{i}|$. The remaining integrals in Eq. (86) just determine in a standard way the usual influence phase for a harmonic bath. In the classical and quantum-mechanical case one obtains the following final result for the partition function:

$$Q(\beta)=Q_{\mathrm{HB}}(\beta)\bar{Q}_N(\beta)\langle e^{(S_0)_B+S_{\mathrm{HB}}}\rangle_N \ . \tag{87}$$

Here Q_{HB} is the partition function for H_{HB}, $\bar{Q}_N$ the partition function for $\bar{H}_N$, and $\langle\cdots\rangle_N$ an average with respect to $\bar{H}_N$ according to Eq. (15). The well-known influence phase S_{HB} for a linear coupling of a harmonic bath is defined and shortly discussed in Sec. V B. The two influence functionals appearing just as a product in Eq. (87) reflect only the fact that we started from dressed states, i.e., from a tensor product of spaces. Specific models of the block decomposition via the K_i operators lead to specific examples for $(S_0)_B$ in Eq. (87). In Ref. 5 we will discuss a calculation of the complicated path in-

tegral $\langle \cdots \rangle_N$ by variational techniques. This possibility makes Eq. (87) a very practical tool to determine partition functions.

We remark that there is also another way to obtain Eq. (87), namely, by reduction step by step. We might first carry out the reduction of the harmonic bath and in the second step contract the K_i blocks. Then we would obtain in the quantum-mechanical case after the first step a Hamiltonian which depends on imaginary time, namely, $H_0+H_I(\{X(\tau)\})$. But our general theory in Sec. II A enables us also to work out the block reduction starting from this time-dependent Hamiltonian.

B. Review of the idea of an influence phase for a harmonic bath

A derivation of the influence phase $S_{\rm HB}$ can be found in many places.[1,2,10–12] Therefore we fix here only our notation and discuss some aspects which we will use. The value of the influence phase $S_{\rm HB}$, Eq. (87), for a path $|\bar{b}^{(\alpha)}\rangle$, $\alpha=0,\ldots,P$, in the reduced state space is (in discretized form)

$$S_{\rm HB}[b^{(\alpha)}]=\frac{1}{P^2}\sum_{\alpha,\alpha'=0}^{P-1}\beta s_{b^{(\alpha)},b^{(\alpha')}}Z_{b^{(\alpha)},b^{(\alpha')}}\left[\frac{|\alpha-\alpha'|}{P}\right] . \tag{88}$$

Here $s_{i,l}$ is the scalar product of the two transition vectors from state i and state l to the harmonic bath,

$$s_{i,l}=\mathbf{c}_i\cdot\mathbf{c}_l \quad \text{with } \mathbf{c}_i\equiv\left[\frac{c_{i,j}}{(2M_j\omega_j^2)^{1/2}}\right]_{j=1,\ldots,J} . \tag{89}$$

The memory function $Z_{i,l}(\tau)$ is identical to 1 in the case of a classical harmonic bath and in the quantum-mechanical case is

$$Z_{i,l}(\tau)\equiv\int_0^\infty \frac{x\cosh[(1-2\tau)x]}{\sinh(x)}\varphi_{i,l}(x)dx , \tag{90a}$$

with the density

$$\varphi_{i,l}(x)\equiv\frac{1}{s_{i,l}}\sum_{j=1}^{J}\frac{c_{i,j}c_{l,j}}{2M_j\omega_j^2}\delta\left[x-\frac{\beta\hbar\omega_j}{2}\right] . \tag{90b}$$

Using Gaussian integrals the memory $\beta s_{i,l}Z_{i,l}(\tau)$ can be written as the time correlation of the matrix elements of the interaction H_I with respect to the harmonic bath,[13]

$$\beta s_{i,l}Z_{i,l}(\tau)=\frac{\beta^2}{2}\langle Y_i(0)Y_l(-i\tau\beta\hbar)\rangle_{H_{\rm HB}} , \tag{91a}$$

where

$$Y_i\equiv\sum_{j=1}^{J}c_{ij}X_j . \tag{91b}$$

This formula is the basis for an interpretation of $\beta s_{i,l}Z_{i,l}(\tau)$ as a response function.[2(b)] In Sec. VI we will derive a similar result for the memory $Y(\tau)$, Eqs. (60) and (78). In the classical case Eq. (91) shows that $S_{\rm HB}^{\rm cl}$ describes the dispersion of the time-averaged interaction $H_I(\{X\})$ with respect to the classical harmonic bath. Equation (88) makes it easy to compare the classical and the quantum-mechanical case: The memory $Z_{i,l}$ corrects the classical influence phase to a quantum-mechanical one. One can demonstrate that one gets in the quantum case in a certain sense the best classical approximation if one replaces $Z_{i,l}$ by 1. $Z_{i,l}(\tau)$ fulfills the sum rule that its integral from 0 to 1 is just 1. Therefore

$$\int_0^1[\xi-\beta s_{i,l}Z_{i,l}(\tau)]^2d\tau=\text{minimum}\Longleftrightarrow\xi=\beta s_{i,l} . \tag{92}$$

We will discuss later how to obtain even better classical approximations for $S_{\rm HB}^{\rm qu}$ by iterative variational procedures. But Eq. (92) allows us to consider neglect of the memory $Z_{i,l}$ as a good starting point.

There is a similarity in the form of the memory $Z_{i,l}$, Eq. (90), and the form of $s_{i,l}$, Eq. (89). $s_{i,l}Z_{i,l}(\tau)$ can be obtained from formula (89) for $s_{i,l}$ if the frequencies $x_j\equiv\beta\hbar\omega_j$ are allowed to vary in time. Setting

$$x_j'(\tau)\equiv\left[\frac{2x_j\sinh(x_j/2)}{\cosh[(1-2\tau)x_j/2]}\right]^{1/2} , \tag{93}$$

one gets

$$s_{i,l}(\{x_j'(\tau)\})=s_{i,l}(\{x_j\})Z_{i,l}(\tau) . \tag{94}$$

Because of the shape of the cosh graph the new frequencies $x_j'(\tau)$ have the square root of $2x_j\tanh(x_j/2)$ as the lower bound and the square root of $2x_j\sinh(x_j/2)$ as the upper bound. For small frequencies x_j, i.e., in the nearly adiabatic case where one can expand all expressions in first order in the x_j's, these bounds of the time-dependent frequencies $x_j'(\tau)$ are very narrow and good values from the classical approximation can be expected.

Further, we remark that the memory function $Z_{i,l}(\tau)$ goes to $\delta(\tau)+\delta(1-\tau)$ for a monochromatic harmonic bath if the frequency goes to infinity. This results from the sum rule for $Z_{i,l}$ together with the Tauberian theorem for Laplace-transformed functions.

Our main interest in comparing the classical and quantum cases is to demonstrate that the calculation of finitely many Gaussian integrals solves the first case whereas the other requires the evaluation of infinitely many Gaussian integrals, which cannot be done on a computer. Therefore here we work out the main features of the classical harmonic bath which is coupled linearly to a system. In Eq. (88) (with $Z_{i,l}\equiv1$) the coordinates X_j *and* the momenta P_j are reduced. More important for us is a form where the coordinates are not yet reduced,

$$e^{S_{\rm HB}^{\rm cl}}=\left\langle\exp\left[-\sum_{j=1}^{J}\frac{1}{P}\sum_{\alpha=0}^{P-1}2x_jd_{b^{(\alpha)},j}\right]\right\rangle_{\{x\}} . \tag{95}$$

Here we use the abbreviation

$$d_{i,j}\equiv\sqrt{\beta}c_{i,j}/(2M_j\omega_j^2)^{1/2} \tag{96}$$

and $\langle\cdots\rangle_{\{x\}}$ means Gaussian averages,

$$\langle f(\{x\})\rangle_{\{x\}}=\pi^{-J/2}\int_{-\infty}^{\infty}dx_1\cdots\int_{-\infty}^{\infty}dx_Je^{-x_1^2-\cdots-x_J^2}\times f(\{x\}) . \tag{97}$$

The procedure to gain Eq. (95) from Eq. (88) is called decompleting the square,[6] namely, decompleting the sca-

lar product Eq. (89). This yields the formula to determine the partition function of the total Hamiltonian H, Eq. (81), by (numerical) matrix diagonalization and forming J Gaussian integrals,

$$Q(\beta)=Q_{\mathrm{HB}}^{\mathrm{cl}}(\beta)\langle \mathrm{Tr}e^{-\tilde{H}}\rangle_{|x|} , \tag{98}$$

where the Hamiltonian $\tilde{H}$ depends on J Gaussian fields

$$\tilde{H}=\beta H_0+\sum_{j=1}^{J} 2x_j D_j \tag{99}$$

and

$$D_j=\sum_{i=1}^{N} d_{i,j}K_i . \tag{100}$$

In fact sometimes even fewer than J Gaussian fields are quite sufficient. N Gaussian fields are enough in any case to fulfill Eq. (98). This works because the influence phase S_{HB}, Eq. (88), is in the classical case totally determined by the scalar products of the vectors $\mathbf{c}_i$, Eq. (89), or of the vectors $\mathbf{d}_i$, Eq. (96). But these N vectors span a space of dimension $J'\le N$. The construction of an orthonormal basis for this space shows, of course, that N vectors $\mathbf{d}_i'$, $i=1,\ldots,N$, in a J'-dimensional space are enough to obtain all $\beta s_{i,l}$ as the scalar product of $\mathbf{d}_i'$ and $\mathbf{d}_l'$. Then Eq. (98) is true if we replace J by J' and D_j by D_j' in Eq. (99) and d_{ij} by $d_{i,j}'$ in Eq. (100) and if we renormalize the frequencies ω_j, $j=1,\ldots,J'$, so that the partition function $Q_{\mathrm{HB}}^{\mathrm{cl}}$ is not changed. This phenomenon can easily be understood considering the fact that there are classes of harmonic baths which deliver after reduction an identical influence on a system. On the other hand, we remark that formal use of Eq. (88) with an arbitrary set of $s_{i,l}$ parameters does not necessarily describe a harmonic bath because the scalar product form, Eq. (89), requires certain constraints, e.g., that the Cauchy-Schwarz inequality

$$s_{i,l}^2\le s_{i,i}s_{l,l} \tag{101}$$

is fulfilled. Nevertheless, one can obtain Eq. (98) from Eq. (88) also be disregarding such conditions on the s parameters, but this may lead to more than N Gaussian ghost fields and even to complex matrices D_j, Eq. (99).

VI. TWO GENERAL EXAMPLES: STATISTICALLY CHARACTERIZED LEVELS AND BRIDGE ASSISTANCE

A. Reduction to a finite basis

From Sec. V, Eq. (87), we know that an explicit formula for the influence phase $(S_0)_B$ of a block decomposition is quite sufficient to obtain a complete result together with a reduction of a harmonic bath. In Sec. IV we already encountered some special examples of influence phases for block decompositions. Here we will develop two examples which are general enough to cover a large variety of applications. Assume that $\{|\sigma\rangle\,|\,\sigma=1,2,\ldots\}$ is an orthonormal basis of an original state space. The original space might be finite dimensional or the dimension might be infinity. A fixed $N\in\mathbb{N}$ is given so that the first $N_1=N-1$ states are called primary and the rest is called secondary. The secondary states shall be reduced whereas the primary states shall be kept unchanged. Therefore we define a partitioning of the state space by the projectors

$$K_i\equiv |i\rangle\langle i| \quad \text{for } i=1,\ldots,N-1 , \tag{102a}$$

$$K_N\equiv Id-\sum_{i=1}^{N-1} K_i . \tag{102b}$$

The Hamiltonian H of the system is assumed to be given in a matrix representation in the given basis. From the decomposition of the basis in primary and secondary states follows a decomposition of H in a primary and a secondary block H_{primary} and H_{sec} and an interaction part $\underline{\mathbf{t}}+\underline{\mathbf{t}}^{\dagger}$ between them,

$$H_{\mathrm{primary}}=\sum_{i,l=1}^{N-1} h_{i,l}\,|i\rangle\langle l|, \quad \text{a } (N-1)^2 \text{ matrix} \tag{103a}$$

$$H_{\mathrm{sec}}=\sum_{i,l=N}^{(\infty)} h_{i,l}\,|i\rangle\langle l| , \tag{103b}$$

$$\underline{\mathbf{t}}=\sum_{i=1}^{N-1}\left[\,|i\rangle\left[\sum_{l=N}^{(\infty)} t_{i,l}\langle l|\right]\right] . \tag{103c}$$

Here $h_{i,l}$ and $t_{i,l}$ denote just the matrix elements of H. We define the reduced space as the direct sum $(\oplus_{i=1}^{N-1}\mathbb{C}\,|\,i\rangle)\oplus\mathbb{C}$ and the reduced Hamiltonian $\overline{H}_N$ as

$$\overline{H}_N\equiv H_{\mathrm{primary}}-\sum_{i=1}^{N-1}(z_i\,|\,i\rangle\langle\overline{N}|+z_i^*\,|\,\overline{N}\rangle\langle i|) +h_{\mathrm{sec}}\,|\,\overline{N}\rangle\langle\overline{N}| , \tag{104}$$

with arbitrary parameters $z_1,\ldots,z_{N-1}\in\mathbb{C}$ and $h_{\mathrm{sec}}\in\mathbb{R}$. For $N=2$ we obtain just the one-fermion problem, Sec. IV B. The proper method to solve the reduction here is an easy generalization of the method used in the one-fermion example. Let us consider the parts H_i and $T_{i,l}$, Eq. (6) of the Hamiltonian H. For $i=1,\ldots,N-1$, H_i vanishes, and H_N is a modification of H_{sec},

$$H_N=H_{\mathrm{sec}}-h_{\mathrm{sec}}K_N . \tag{105}$$

For $i,l<N$ the transition operators $T_{i,l}$ are simply $|i\rangle\langle l|$ and for $i<l=N$ we obtain with the transition vector $\langle i\,|\,\underline{\mathbf{t}}$,

$$T_{i,N}=-\,|i\rangle\frac{\langle i\,|\,\underline{\mathbf{t}}}{z_i} . \tag{106}$$

Therefore all i,l lead to separable transitions $T_{i,l}$ and the influence phase S_B for the block decomposition can be described by memory functions

$$Y_{i,l}(\tau)\equiv\ln(\langle i\,|\,\underline{\mathbf{t}}e^{-\tau\beta H_N}\underline{\mathbf{t}}^{\dagger}\,|\,l\rangle/z_i z_l^*) . \tag{107}$$

Thus we get for the complicated part $S_{\mathrm{sec}}\equiv S_B^0$, Eq. (40), the form

$$S_{\mathrm{sec}}[b^{(\alpha)}]=\sum_{k=0}^{P-2}\sum_{\alpha=0}^{P-1} Y_{b^{(\alpha)},b^{(\alpha+k+2)}}\left[\frac{k}{P}\right](1-\bar{n}_N^{(\alpha)}) \times\prod_{\gamma=1}^{k+1}\bar{n}_N^{(\alpha+\gamma)}(1-\bar{n}_N^{(\alpha+k+2)}) , \tag{108}$$

where $|\bar{b}^{(\alpha)}\rangle$, $\alpha=0,\ldots,P-1$, is a path in the reduced space $\mathbb{C}^N$ and $\bar{n}_i^{(\alpha)}=\langle \bar{i}\,|\,\bar{b}^{(\alpha)}\rangle$ are occupation numbers. Comparison of this result with Eq. (61) in the one-fermion example shows clearly how the generalization is performed. The indices i,l of the memory functions $Y_{i,l}$ keep track of the fact that we have in general more than one primary state. The indices solve the additional combinatorial problem. The same trick is already used by the construction of the harmonic-bath influence phase with the indices of the memory function $Z_{i,l}(\tau)$, Eq. (88).

The eigenvector part S_{EV}, Eq. (39), is

$$S_{\mathrm{EV}}[b^{(\alpha)}]=\ln(\mathrm{Tr}_{\mathrm{sec}}e^{-\beta H_N})\prod_{\alpha=0}^{P-1}\bar{n}_N^{(\alpha)}\ . \tag{109}$$

It contributes only for the path where the system is trapped in the secondary states. With Eqs. (108) and (109) the influence phase S_B for the block decomposition is fully determined. In Sec. III C we discussed the possibility of including the eigenvector part S_{EV} in a trivial extension of the reduced Hamiltonian $\bar{H}_N$ with the consequence that the system is completely solvable by a finite (small) matrix diagonalization if the memory S_{sec} vanishes.

Now we discuss some properties of the memory functions $Y_{i,l}(\tau)$. Expansion of $Y_{i,l}(\tau)$ in a power series in τ shows that all memories $Y_{i,l}$ vanish identically if and only if the following two conditions are fulfilled:

$$\langle i|\underline{\mathbf{t}}\,\underline{\mathbf{t}}^{\dagger}|l\rangle=z_i z_l^{*}\quad\text{for all } i,l\ , \tag{110a}$$

$$\underline{\mathbf{t}}H_N^{n}\underline{\mathbf{t}}^{\dagger}=0\quad\text{for all } n\geq 1\ . \tag{110b}$$

Equation (110a) is equivalent to $Y_{i,l}(0)=0$ and it contains the condition that the absolute value $|z_i|$ norms the transition vectors $\langle i|\underline{\mathbf{t}}$. This means that the transition matrices $T_{i,N}$ are not only separable but also permutation-like. This algebraic condition is not surprising from our earlier observation comparing Eqs. (21) and (22) that the transition matrices $T_{i,N}$ are represented after reduction by the raising operators $|i\rangle\langle\bar{N}|$. This suggests that setting $z_i=|\langle i|\underline{\mathbf{t}}|$ is a good *a priori* choice for the parameters z_i. Having in mind to also minimize the first-order moment of $Y_{i,l}(\tau)$ leads from Eq. (110b) with $n=1$ to an *a priori* choice of h_{sec} as the arithmetic average of the quadratic forms $(\langle i|\underline{\mathbf{t}})^{0}\beta H_{\mathrm{sec}}(\langle i|\underline{\mathbf{t}})^{\dagger 0}$, where the superscript 0 indicates normalization of the vectors. These observations are useful for obtaining proper starting values for the variational procedures discussed in the following paper.

Now assume z_i to be the norm of the vector $\langle i\,|\,\underline{\mathbf{t}}$. Then the operators $K_N^{(i)}$ defined in Sec. III A are projectors on the space of secondary states. With the aid of these projectors we get a possibility to interpret the memory functions $Y_{i,l}$ as two-point two-time correlation functions similar to the interpretation of the memory functions $Z_{i,l}$ for a harmonic bath according to Eq. (91).

$$Y_{i,l}(\tau)+Y_{i,l}^{*}(1-\tau)=\ln(\mathrm{Tr}e^{-\beta H_N})+\ln(\langle K_N^{(i)}K_N^{(l)}(-i\tau\beta\hbar)\rangle_{H_N})\ . \tag{111}$$

As in the harmonic-bath case the right-hand side of Eq. (111) contains the secondary-part average of the time correlation of coupling operators, operating only on the space of secondary states. But in contrast to the harmonic-bath case only the combination $Y_{i,l}(\tau)+Y_{i,l}^{*}(1-\tau)$ has this property, not $Y_{i,l}(\tau)$ alone. This is easily understood because the entire memory, Eq. (108), contains not only the memory functions $Y_{i,l}$ but also the long-range (in time) product of the occupation numbers $\bar{n}_N$, namely, the path test. This path test distinguishes the contribution of the path and the reverse path, whereas in the harmonic-bath case a path and its reverse have the same Boltzmann weight. We remark that a formula similar to Eq. (111) is true for the real part of $Y_{i,l}(\tau)$. The imaginary part of $Y_{i,l}(\tau)$ can be written, however, with a quotient of two different correlation functions.

In order to make Eq. (108) useful for numerical calculations, such as variational procedures, one should note that S_{sec} has as ingredients besides the memory functions $Y_{i,l}$ a characteristic structure. Therefore one can use models for the memory functions $Y_{i,l}$ starting from physical arguments instead of straightforward insertion of the matrices $\underline{\mathbf{t}}$ and H_N in the definition, Eq. (107). Then our theory is a real help to correct finite basis calculations, such as Hartree-Fock calculations by a model for the remaining influence of the rest. In Sec. VI B, we will discuss such a modeling of the Y functions under some specific assumptions. Besides truncation of a basis we will demonstrate another application of our developments. Assume two chemical compounds, such as chromophores, are connected by a bridge and one is interested in the influence of the bridge (secondary states) on the two compounds (primary states). Our formalism allows us to contract the bridge to *one* additional state and a memory. By variational procedures we can then renormalize the system so that it contains most of the influence of the bridge. In Sec. VI C we will extend this example to the case of two competing bridges.

B. Modeling of memory functions from a random-noise argument

The discussion thus far has considered mostly fermion systems, but the idea of influence functionals is equally powerful in the boson case. We consider now a situation in which a set of energy levels of primary interest is coupled to another, larger set of levels about which only statistical information, such as the mean spacing of the levels, is available. Examples include energy levels in nuclei,[15,16] in small metal particles,[17] and in molecular vibrations.[18]

We start again from the Hamiltonian H, Eq. (103), and the partitioning due to Eq. (102) but the given basis $\{|\sigma\rangle\}$ should be constructed so that the parts H_{primary} and H_{sec} are diagonal in this basis,

$$H_{\mathrm{primary}}=\sum_{i=1}^{N-1}\lambda_i\,|\,i\rangle\langle i\,|\ , \tag{112a}$$

$$H_{\mathrm{sec}}=\sum_{i=1}^{M}E_i\,|\,N-1+i\rangle\langle N-1+i\,|\ . \tag{112b}$$

One might think of a few $(N-1)$ main vibrational levels λ_i coupled via $\underline{t}$ to a larger number (M) of uncertain vibrational levels E_l and we will study the influence of the statistically described levels E_l on the levels λ_i. The influence phase S_B is given according to Eqs. (108) and (109) but now the coefficients have a special form,

$$\ln(\mathrm{Tr}_{\mathrm{sec}} e^{-\beta H_N}) = \ln \sum_{m=1}^{M} e^{-\beta E_m} , \tag{113a}$$

$$Y_{i,l}(\tau) = \ln \left[\sum_{m=1}^{M} \frac{\langle i \,|\, \underline{t} \,|\, N-1+m \rangle \langle l \,|\, \underline{t} \,|\, N-1+m \rangle^*}{z_i z_l^*} \times e^{-\tau\beta E_m} \right] , \tag{113b}$$

where we have used the reduced Hamiltonian $\overline{H}_N$ as in Eq. (104) but with $h_{\mathrm{sec}}=0$. The m sum extends over all secondary states but the exponential factor $e^{-\tau\beta E_m}$ depends only on the energy E_m of the mth secondary state. Doing the sum over degeneracies first, we obtain the following result, which is the exact analogue to Eq. (90) in the harmonic-bath case,

$$Y_{i,l}(\tau) = Y_{i,l}(0) + \ln \left[\int_{-\infty}^{\infty} e^{-\tau\beta E} \underline{\rho}_{i,l}(E) dE \right] , \tag{114a}$$

with the density

$$\underline{\rho}_{i,l}(E) = \sum_{m=1}^{M} \frac{\langle i \,|\, \underline{t} \,|\, N-1+m \rangle \langle l \,|\, \underline{t} \,|\, N-1+m \rangle^*}{\langle i \,|\, \underline{t}\,\underline{t}^{\dagger} \,|\, l \rangle} \times \delta(E - E_m) . \tag{114b}$$

This means that $\exp[Y_{i,l}(\tau)]$ is, up to the norm factor $\exp[Y_{i,l}(0)]$, the Laplace transform of the density $\underline{\rho}_{i,l}(E)$.

As in the harmonic bath case[14] it remains to give a model for the densities $\underline{\rho}_{i,l}$. First we remark that in the monochromatic case, i.e., if $E_m = E_1$ for all m, $\underline{\rho}_{i,l}$ is a simple δ function $\delta(E-E_1)$ and therefore the memory $Y_{i,l}(\tau)$ is linear in τ. In general we proceed here with an assumption which allows us to discuss coupling and energy distribution of the secondary part separately. Let

$$\langle i \,|\, \underline{t} \,|\, N-1+m \rangle = z_i f_i(E_m) \quad \text{with a function } f_i , \tag{115}$$

i.e., the coupling matrix element $\langle i \,|\, \underline{t} \,|\, N-1+m \rangle$ varies—as is true for the exponential factor $e^{-\tau\beta E_m}$—via its energy *only*. A reasonable form for the function $f_i(E)$ is a gap law $\exp(-a_i \,|\, \lambda_i - E \,|\,)$. With Eq. (115) one obtains for the memory function

$$Y_{i,l}(\tau) = \ln \left[\int_{-\infty}^{\infty} f_i(E) f_l^*(E) e^{-\tau\beta E} \mu(E) dE \right] , \tag{116}$$

where $\mu(E)/M$ is just the density of states with energy E. The norm factor $\exp[Y_{i,l}(0)]$ is here the scalar product of the two coupling functions f_i and f_l with the weight μ. The norm of $\langle i \,|\, \underline{t}$ divided by $|\, z_i \,|$ delivers the μ norm of the function f_i. It is of course easier to model the functions f_i and the weight μ separately because their physical meaning is clear. From the assumption of degenerate oscillators we obtain the following continuous model for μ:

$$\mu(E) = \frac{1}{\hbar\omega} \frac{(E/\hbar\omega)^{s-1}}{(s-1)!} \chi_{[0,E_0]}(E) . \tag{117}$$

Here ω is the frequency of the oscillators, s is the number of modes, and E_0 the dissociation energy. The characteristic function $\chi_{[0,E_0]}$ is 1 on the interval $[0,E_0]$ and 0 otherwise. Inserting the model, Eq. (117), and exponential coupling functions f_i as given above, the integral defining $Y_{i,l}(\tau)$ in Eq. (116) can be done immediately by the truncated γ functions and these functions are, for natural numbers s, easily expressed by exponential functions and truncated exponential functions. So we obtained a model for the memory functions which can immediately be calculated from simple exponential functions and a logarithm. But Eq. (117) is not the only possibility to model the density of states $\mu(E)/M$. Numerically given power laws can be inserted in Eq. (116) and with our formalism we get a method to test such models by looking at the influence resulting from it. Furthermore, the sensitivity to different algebraic forms of the density of states can be tested. We remark that beyond the density of states of the statistical part of the Hamiltonian, one can, as in Eq. (114a), derive a formula for the memory $Y_{i,l}(\tau)$ using the joint distribution of the eigenvalues of the secondary part. But then one has to evaluate multifold integrals. Nevertheless, this shows a way to perform joint distributions derived for certain matrix ensembles[15] which may be useful in the physical context of a large (statistical) secondary system.

C. Two competing bridges

There is very widespread interest in electron transfer between two localization sites via a bridging structure; examples include superexchange coupling and mixed valence in binuclear metal complexes,[19] through-bond transfer in proteins,[20] and bridge-assisted transfer in general.[21] We will approach the purely electronic aspects of this problem of bridge assistance using the reduction of the effective Hamiltonian and construction of S_{EV} and of S^0.

As in Sec. VI A let $|\, \sigma \rangle$, $\sigma = 1,2,\ldots$, be an orthonormal basis of an original space but now we take a partitioning of the basis following the idea that the first $N_1 = N-2$ states describe a system of two chemical compounds. The next N_2 states $|\, N-1 \rangle, \ldots, |\, N-2+N_2 \rangle$ describe a first bridge between the two systems and the remaining N_3 states describe a second bridge between the two compounds. Our aim is to contract the two bridges separately. Therefore we define projectors K_i by

$$\begin{aligned} K_i &\equiv |\, i \rangle \langle i \,| \quad \text{for } i = 1,\ldots,N-2 , \\ K_{N-1} &\equiv \sum_{i=N-1}^{N-2+N_2} |\, i \rangle \langle i \,| , \\ K_N &\equiv \sum_{i=N-1+N_2}^{N-2+N_2+N_3} |\, i \rangle \langle i \,| . \end{aligned} \tag{118}$$

We assume that the two bridges compete only, i.e., they are not coupled among one another. They are only coupled to the systems. Thus we get the following decompo-

sition of the matrix representation of the Hamiltonian H:

$$H=\begin{bmatrix} H_{\text{primary}} & \underline{t}^{(1)} & \underline{t}^{(2)} \\ \underline{t}^{(1)\dagger} & H^{(1)} & 0 \\ \underline{t}^{(2)\dagger} & 0 & H^{(2)} \end{bmatrix} . \tag{119}$$

Here the superscripts 1 and 2 denote the first and the second bridge, respectively. $H^{(1)}$ has N_2 lines and $H^{(2)}$ has N_3 lines. To reduce the two bridges separately we define the reduced Hamiltonian $\overline{H}_N$ as

$$\overline{H}_N \equiv H_{\text{primary}} - \left[\sum_{i=1}^{N-2} (z_{1,i} \mid i\rangle\langle \overline{N-1} \mid + z_{2,i} \mid i\rangle\langle \overline{N} \mid) + \text{adjoint} \right] + h^{(1)} \mid \overline{N-1}\rangle\langle \overline{N-1} \mid + h^{(2)} \mid \overline{N}\rangle\langle \overline{N} \mid . \tag{120}$$

The method of solving the reduction problem is the same as in Sec. VI A and shall therefore not be repeated here. Besides that all quantities occur twofold, namely, for every bridge, the only complication is the existence of a different transition matrix $T_{N-1,N}$. But a transition between the two bridges is forbidden and therefore according to our general theory, Eqs. (4) and (6), $T_{N-1,N}$ can be chosen arbitrarily. So we obtain for the influence phase

$$S_B = S_{\text{EV}}^{(1)} + S_{\text{EV}}^{(2)} + S_{\text{sec}}^{(1)} + S_{\text{sec}}^{(2)} , \tag{121a}$$

with

$$S_{\text{EV}}^{(\nu)}[b^{(\alpha)}] = \ln(\text{Tr}^{(\nu)} e^{-\beta H_{N-2+\nu}}) \prod_{\alpha=0}^{P-1} \overline{n}_{N-2+\nu}^{(\alpha)} , \tag{121b}$$

$$S_{\text{sec}}^{(\nu)}[b^{(\alpha)}] = \sum_{k=0}^{P-2} \sum_{\alpha=0}^{P-1} Y_{b^{(\alpha)},b^{(\alpha+k+2)}}^{(\nu)} \left[\frac{k}{P} \right] (1-\overline{n}_{N-2+\nu}^{(\alpha)}) \times \prod_{\gamma=1}^{k+1} \overline{n}_{N-2+\nu}^{(\alpha+\gamma)} (1-\overline{n}_{N-2+\nu}^{(\alpha+k+2)}) . \tag{121c}$$

The memory functions $Y_{i,l}^{(\nu)}$ are

$$Y_{i,l}^{(\nu)}(\tau) = \ln(\langle i \mid \underline{t}^{(\nu)} e^{-\tau\beta H_{N-2+\nu}} \underline{t}^{(\nu)\dagger} \mid l\rangle / z_{\nu,i} z_{\nu,l}^{*}) . \tag{122}$$

Of course, it is a fact that the two bridges are uncoupled and the reduction problem is solvable along the lines of Sec. VI A. The problem is also solvable for coupled bridges if the two bridges are equivalent in the sense $H^{(1)} \cong H^{(2)} + \eta K_N$, and the coupling leads to a permutationlike transition which permutes only $H^{(1)}$ and $H^{(2)}$. A special example for this case is the four states two electron problem of Sec. IV C. It is obvious that also three and more uncoupled bridges can be treated with our formalism.

VII. CONCLUSIONS

Starting from a general observation, the construction of discretized path integrals for operators with the help of Trotter's product formula, we developed a formalism to write down influence functionals for a large class of problems explicitly. In a variety of special and general examples, we have demonstrated that the formalism can be applied successfully and yields many new insights. Two sorts of influence functionals are considered, one corresponding to a heat bath, the second to a second subsystem coupled directly to the subsystem of primary interest. The reduction of a heat bath formulated traditionally as a harmonic bath is a possibility to describe the statistical effect of a system coupled to an environment. Reduction of a block structure of a Hamiltonian is a natural way to introduce either a distribution of only statistically known levels around the levels of the main spectrum, or the effects of one subset of levels, such as a bridge or a manifold of electronic states, on the system being described. Considering once again Eq. (42) and the following discussion we see how lifetimes of (reduced) levels can be extracted from reduction of a block structure.

The formalism presented works in real time as well as in imaginary time. But the statistical, purely temperature-dependent problem can be solved numerically in a very effective way by a variational procedure, whereas the *real* time-dependent problem does not permit such an easy way to calculate partition functions and correlation functions. In real time, path integrals usually have to be evaluated by Monte Carlo techniques. In a second, very formal paper we will derive all the equations in analytic form which enables us to calculate partition functions variationally in the imaginary-time case starting from the general examples of Sec. VI.

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