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Open Quantum Systems with Time-Dependent Hamiltonians and Their Linear Response

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We give a rigorous (Hamiltonian) treatment of a quantum system weakly coupled to an infinite free reservoir and subject to an external time-dependent driving potential varying on the scale of dissipation. The linear response of the system initially in thermal equilibrium is determined and compared with the usual expressions of linear response theory.

KEY WORDS: Open quantum systems; time-dependent Hamiltonians; linear response.

1. INTRODUCTION

Linear response theory[1–3] gives a supposedly universal prescription for the computation of transport coefficients in the linear regime (i.e., where the fluxes depend linearly on the driving forces). They are expressed in terms of time integrals over certain time-dependent equilibrium correlation functions. However, for a finite, closed system the prescription makes no sense, for physically well-understood reasons. For a classical system the result obtained is typically zero,[4] for a quantum system the correlation functions are almost periodic functions of time, and hence, in general, the time integrals will not exist. Usually, therefore, one assumes[3] that the time integrals should be computed over the correlation functions of the infinitely extended system, i.e., one should first take the thermodynamic (infinite-volume) limit and then the limit as time goes to infinity. (For some results in this direction see Refs. 5 and 6.) An alternative modification is to place the finite system in idealized isothermal surroundings.[7] This should induce sufficient decay of

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the correlation functions for the time integrals to exist. In the limit of a large system the transport coefficients computed in this manner should coincide with those obtained from the previous method.

The goal of the present paper is to give a rigorous Hamiltonian formulation of the second approach. We consider a quantum system with Hamiltonian H coupled to an infinitely extended ideal Fermi gas and subject to a time-dependent driving potential $f(t)A$. We assume a weak coupling to the reservoir (at present, this is the only case which can be handled). For obvious reasons the driving potential has to vary on the time scale of the dissipation processes induced by the reservoir. We start by extending the weak coupling theory[8,9] to time-dependent Hamiltonians. With this tool in hand we investigate the linear response of the system initially in thermal equilibrium. The result differs somewhat from the naive expectation. The "off-diagonal response" (with respect to the time-independent system Hamiltonian H) follows instantaneously the driving force, whereas the "diagonal response" has the usual form, provided that the Hamiltonian dynamics of the isolated system is replaced by a stochastic time evolution given in terms of a quantum dynamical semigroup, which is obtained in the weak coupling limit (in the interaction picture) with the Hamiltonian H.

We remark that the case of nonmechanical, time-independent perturbations (e.g., temperature gradients) is treated in Ref. 10.

2. DESCRIPTION OF THE MODEL

We consider a quantum system specified by a finite-dimensional Hilbert space $\mathscr{H}$ and a time-dependent Hamiltonian H_t, where the time dependence arises from an external field acting on the system. For technical reasons we assume that H_t is a real, analytic function of t. The system is coupled to an infinite, quasi-free fermion reservoir with Hilbert space $\mathscr{F}$, Hamiltonian F, and stationary state Ω, so that $F\Omega = 0$. We take the Hamiltonian of the system plus reservoir to be of the form

$$H_t^\lambda = H_{\lambda^2 t} + F + \lambda H_I$$

where the interaction term

$$H_I = \sum_{r=1}^{N} Q_r \otimes \phi_r$$

is bounded, the ϕ_r being linear, smeared fermion operators on $\mathscr{F}$ with $\langle \phi_r \Omega, \Omega \rangle = 0$. We assume Q_r and ϕ_r are self-adjoint without loss of generality.

We consider the time evolution of the system in the weak coupling and adiabatic limit $\lambda \to 0$ by adapting the methods of Refs. 8 and 9. We define

$\mathscr{B}$ to be the Banach space of trace class operators on $\mathscr{H} \otimes \mathscr{F}$, and $\mathscr{B}_0$ to be the Banach space of trace class operators on $\mathscr{H}$, identifying $\mathscr{B}_0$ as a subspace of $\mathscr{B}$ by the one–one correspondence $\rho \leftrightarrow \rho \otimes v$, where $v = |\Omega\rangle\langle\Omega|$. We let P_0 be the partial trace with respect to $\mathscr{F}$, so that it is a projection of $\mathscr{B}$ onto $\mathscr{B}_0$, and put $P_1 = 1 - P_0$ and $\mathscr{B}_1 = P_1\mathscr{B}$.

After rescaling the time variable by the factor λ^2, we find for the evolution equation of a state ρ on $\mathscr{B}$

$$d\rho/dt = [\lambda^{-2}Z(t) + \lambda^{-1}A]\rho \tag{1}$$

where

$$Z(t)\rho = -i[H_t + F, \rho], \qquad A\rho = -i[H_I, \rho]$$

We observe that $Z(t)$ commutes with P_0 and that if we define $A_{ij} = P_iAP_j$, then $A_{00} = 0$.

Although time-dependent evolution equations are known to be difficult to interpret rigorously in some circumstances,[11,12] these difficulties do not arise in our case because the time dependence arises from a norm-bounded real analytic term. We can therefore manipulate with the Born series and associated integral equations exactly as in the time-independent case.

Let $V_\lambda(t, s)$ be the propagator on $\mathscr{B}$ associated with (1) and defined for $0 \leqslant s \leqslant t < \infty$, and let $U_\lambda(t, s)$ be the propagator associated with the evolution equation

$$d\rho/dt = [\lambda^{-2}Z(t) + \lambda^{-1}A_{11}]\rho$$

Then $U_\lambda(t, s)$ commutes with P_0 and its restriction to the subspace $\mathscr{B}_0$ is an isometry for all $0 \leqslant s \leqslant t < \infty$. Moreover,

$$V_\lambda(t, s) = U_\lambda(t, s) + \lambda^{-1}\int_s^t du\, U_\lambda(t, u)(A_{01} + A_{10})V_\lambda(u, s)$$

If $f \in \mathscr{B}_0$ and we define the state of the system at time $t \geqslant 0$ by

$$f_\lambda(t) = P_0V_\lambda(t, 0)f$$

then a routine manipulation leads to

$$f_\lambda(t) = U_\lambda(t, 0)f + \int_0^t ds\, U_\lambda(t, s)L(\lambda, t, s)f_\lambda(s) \tag{2}$$

where the operators $L(\lambda, t, s)$ on $\mathscr{B}_0$ are defined by

$$\begin{aligned} L(\lambda, t, s) &= \lambda^{-2}\int_s^t du\, U_\lambda(u, s)^{-1}A_{01}U_\lambda(u, s)A_{10} \\ &= \int_0^{\lambda^{-2}(t-s)} dv\, U_\lambda(s + \lambda^2 v, s)^{-1}A_{01}U_\lambda(s + \lambda^2 v, s)A_{10} \end{aligned}$$

Our analysis of the form of $f_\lambda(t)$ for small λ proceeds in several stages, the first of which is given in the following theorem.

Theorem 1. Suppose that the reservoir two-point functions

$$h_{ij}(t) = \langle e^{iFt}\phi_i e^{-iFt}\phi_j\Omega, \Omega\rangle$$

all satisfy

$$\int_0^\infty dt\, |h_{ij}(t)|(1 + |t|)^\epsilon < \infty$$

for some $\epsilon > 0$. Then there exist operators $L(t)$ on $\mathscr{B}_0$ depending continuously on t, such that if $g_\lambda(t)$ is the solution of the evolution equation

$$\frac{d}{dt} g_\lambda(t) = [\lambda^{-2}Z(t) + L(t)]g_\lambda(t) \tag{3}$$

with initial conditions $g_\lambda(0) = f$, then

$$\lim_{\lambda\to 0} \sup_{0\leqslant t\leqslant t_0} \|g_\lambda(t) - f_\lambda(t)\| = 0 \tag{4}$$

for all $0 \leqslant t_0 < \infty$.

Proof. Since this is only a slight variation upon the corresponding time-independent theorems in Refs. 8 and 9, we content ourselves with some brief comments.

We first note that for all $v, s \geqslant 0$

$$\lim_{\lambda\to 0} U_\lambda(s + \lambda^2 v, s) = e^{Z(s)v}$$

so that in a formal sense

$$\lim_{\lambda\to 0} L(\lambda, t, s) = L(s) \tag{5}$$

where

$$L(s) = \int_0^\infty dv\, e^{-Z(s)v}A_{01}e^{Z(s)v}A_{10} \tag{6}$$

Second, the evolution equation (3) is equivalent to the integral equation

$$g_\lambda(t) = U_\lambda(t, 0)f + \int_0^t ds\, U_\lambda(t, s)L(s)g_\lambda(s) \tag{7}$$

and since both (2) and (7) are of Volterra type, the theorem is obtained as in Refs. 8 and 9 by proving that (5) is rigorously valid in a suitable sense. Moreover, this is achieved exactly as in Refs. 8 and 9, the only difference in the problem being that the system Hamiltonian is time-dependent; this, however, does not matter, because only crude norm estimates of operators on the system space $\mathscr{H}$ are used in Refs. 8 and 9.

It is clear from (6) the $L(s)$ depends continuously on s. ∎

3. THE ADIABATIC LIMIT

We summarize the essential features of the definition of the functions $g_\lambda(t)$. The space $\mathscr{B}_0$ is a finite-dimensional Hilbert space for the Hilbert–Schmidt norm, and for all $t \geqslant 0$, $Z(t)$ is the generator of a one-parameter unitary group on $\mathscr{B}_0$. Moreover, $Z(t)$ is a real, analytic function of t, while $L(t)$ is a continuous function of t. Finally, $g_\lambda(t)$ is the solution of the differential equation

$$g_\lambda'(t) = [\lambda^{-2}Z(t) + L(t)]g_\lambda(t) \tag{8}$$

with initial conditions $g_\lambda(0) = f$. (We use the prime for the derivative with respect to t.) We analyze $g_\lambda(t)$ in the adiabatic limit $\lambda \to 0$, our method being a slight modification of that followed in Refs. 13 and 14.

By Ref. 15, p. 120, the eigenvalues $-i\omega_n(t)$ of $Z(t)$ are analytic and can be continued analytically through accidental degeneracies, which occur only at a discrete set T of times. Moreover, the spectral projections $P_n(t)$, which satisfy

$$\sum_n P_n(t) = 1, \qquad P_n(t)Z(t) = Z(t)P_n(t) = -i\omega_n(t)P_n(t)$$

are also analytic functions which may be continued through points of T. An example in Ref. 15, p. 111, shows that this last property may fail if $Z(t)$ is only a C^∞-function of t.

Lemma 1. If we define

$$K(t) = -\sum_n P_n(t)P_n'(t) \tag{9}$$

then

$$P_n(t)K(t)P_n(t) = 0 \tag{10}$$

and the solution of the differential equation

$$W'(t) = K(t)W(t) \tag{11}$$

with initial conditions $W(0) = 1$, consists of unitary operators $W(t)$ satisfying

$$W(t)P_n(0) = P_n(t)W(t) \tag{12}$$

Proof. Differentiation of

$$P_n(t)^2 = P_n(t) = P_n(t)^*$$

leads to

$$P_n(t)P_n'(t) + P_n'(t)P_n(t) = P_n'(t) = P_n'(t)^*$$

which implies

$$P_n(t)P_n'(t)P_n(t) = 0$$

and hence (10). Moreover,

$$\begin{aligned} K(t)^* &= -\sum_n P_n'(t)^*P_n(t)^* = -\sum_n P_n'(t)P_n(t) \\ &= \sum_n [P_n(t)P_n'(t) - P_n'(t)] = -K(t) - \Big[\sum_n P_n(t)\Big]' \\ &= -K(t) \end{aligned}$$

and this implies that $W(t)$ are unitary. Finally,

$$\begin{aligned} [W(t)^*P_n(t)W(t)]' &= W(t)^*[K(t)^*P_n'(t) + P_n'(t) + P_n(t)K(t)]W(t) \\ &= W(t)^*[-P_n'(t)P_n(t) + P_n'(t) - P_n(t)P_n'(t)]W(t) \\ &= 0 \end{aligned}$$

so

$$W(t)^*P_n(t)W(t) = P_n(0)$$

which leads immediately to (12). ■

Before stating the next theorem we introduce some notation. If $B(t)$ are operators on $\mathscr{B}_0$, we write

$$B(t)^\sim = W(t)^{-1}B(t)W(t), \qquad B(t)^\natural = \sum_n P_n(0)B(t)^\sim P_n(0)$$

Lemma 2. The solution of the differential equation

$$X_\lambda'(t) = \lambda^{-2}Z(t)^\sim X_\lambda(t) \tag{13}$$

with initial conditions $X_\lambda(0) = 1$ is

$$X_\lambda(t) = \sum_n P_n(0)\exp[-i\lambda^{-2}\mu_n(t)] \tag{14}$$

where

$$\mu_n(t) = \int_0^t \omega_n(s)\,ds$$

Proof. This is an immediate deduction from the formula

$$Z(t)^{\sim} = -i \sum_n P_n(0)\omega_n(t) \quad \blacksquare$$

Theorem 2. If $g_\lambda(t)$ is defined by (8), then

$$\lim_{\lambda \to 0} \sup_{0 \leqslant t \leqslant t_0} \| g_\lambda(t) - W(t)Y(t)X_\lambda(t)f \| = 0 \tag{15}$$

for all $0 \leqslant t_0 < \infty$, where $Y(t)$ is the solution of

$$Y'(t) = L(t)^{\natural} Y(t)$$

with initial conditions $Y(0) = 1$.

Proof. We notice that $[Y(t), X_\lambda(t)] = 0$, since

$$Y(t) = \sum_{n=0}^{\infty} \int_{0 \leqslant t_1 \leqslant \cdots \leqslant t_n \leqslant t} dt_n \cdots dt_1 \sum_m P_m(0)L(t_n)^{\sim} P_m(0) \cdots P_m(0)L(t_1)^{\sim} P_m(0)$$

and since, by (14), $X_\lambda(t)$ commutes with every term of this sum. If

$$h_\lambda(t) = X_\lambda(t)^{-1} W(t)^{-1} g_\lambda(t)$$

then

$$\begin{aligned} h_\lambda'(t) &= -\lambda^{-2} Z(t)^{\sim} h_\lambda(t) + X_\lambda(t)^{-1} W(t)^{-1} [\lambda^{-2} Z(t) + K(t)^* + L(t)] g_\lambda(t) \\ &= -\lambda^{-2} Z(t)^{\sim} h_\lambda(t) + X_\lambda(t)^{-1} [\lambda^{-2} Z(t)^{\sim} + K(t)^{*\sim} + L(t)^{\sim}] X_\lambda(t) h_\lambda(t) \\ &= X_\lambda(t)^{-1} [K(t)^{*\sim} + L(t)^{\sim}] X_\lambda(t) h_\lambda(t) \end{aligned}$$

so

$$h_\lambda(t) = f + \int_0^t ds\, X_\lambda(s)^{-1} [K(s)^{*\sim} + L(s)^{\sim}] X_\lambda(s) h_\lambda(s)$$

and we have to show that $h_\lambda(t)$ converges uniformly on $[0, t_0]$ to the solution

$$h(t) = Y(t)f$$

of the integral equation

$$h(t) = f + \int_0^t ds\, L(s)^{\natural} h(s)$$

Since these are Volterra integral equations it is sufficient as in Refs. 8 and 9 to show that the Volterra integral operators $\mathscr{K}_\lambda$ defined on the space $\mathscr{V}$ of continuous functions k: $[0, t_0] \to \mathscr{B}_0$ by

$$(\mathscr{K}_\lambda k)(t) = \int_0^t ds\, \{X_\lambda(s)^{-1} [K(s)^{*\sim} + L(s)^{\sim}] X_\lambda(s) - L(s)^{\natural}\} k(s)$$

converge strongly to zero as $\lambda \to 0$. Using (10) and (14), we see that

$$(\mathscr{H}_\lambda k)(t) = \sum_{m \neq 0} \int_0^t ds\, P_m(0)[K(s)^{*\sim} + L(s)^{\sim}]P_n(0) \\ \times \exp[i\lambda^{-2}\mu_m(s) - i\lambda^{-2}\mu_n(s)]k(s)$$

Density arguments show that it is sufficient to prove that

$$\lim_{\lambda \to 0} \sup_{0 \leqslant t \leqslant t_0} \left| \int_0^t ds \exp[i\lambda^{-2}\mu_m(s) - i\lambda^{-2}\mu_n(s)]p(s) \right| = 0$$

$n \neq m$, for all continuously differentiable functions p whose support does not contain any point of the set T of accidental degeneracies. For such p and $n \neq m$

$$\int_0^t ds \exp[i\lambda^{-2}\mu_m(s) - i\lambda^{-2}\mu_n(s)]p(s)$$

$$= \left\{ -i\lambda^2 \exp[i\lambda^{-2}\mu_m(s) - i\lambda^{-2}\mu_n(s)] \frac{p(s)}{\omega_m(s) - \omega_n(s)} \right\}_0^t$$

$$+ \int_0^t ds\, i\lambda^2 \exp[i\lambda^{-2}\mu_m(s) - i\lambda^{-2}\mu_n(s)] \frac{d}{ds} \left(\frac{p(s)}{\omega_m(s) - \omega_n(s)} \right)$$

$$= O(\lambda^2)$$

as required. ∎

Note. The above theorem reduces to the ordinary adiabatic theorem if $L = 0$, and shows that as $\lambda \to 0$, the entire λ dependence of $g_\lambda(t)$ is effectively concentrated in the single term $X_\lambda(t)$.

4. LINEAR RESPONSE THEORY

Let H be the (time-independent) Hamiltonian of the quantum mechanical system under consideration. We assume that the quasi-free fermion reservoir is in thermal equilibrium, i.e., that Ω is a KMS state with respect to F at inverse temperature β, and, furthermore, that the system is well coupled to its reservoir, in the sense that $\{A | [H, A] = 0, [Q_r, A] = 0, r = 1,..., N\} = \{\mathbb{C}1\}$ and that the Fourier transform $\hat{h}_{ij}(\omega)$ of $h_{ij}(t)$ is strictly positive as a matrix for all points ω in the spectrum of $[H, \cdot]$. This condition ensures that in the weak coupling limit every initial state ρ of the system approaches the canonical equilibrium state $\rho_\beta = e^{-\beta H}/\mathrm{tr}\, e^{-\beta H}$ as $t \to \infty$.[16] The system is assumed to be in equilibrium. At time $t = 0$ a mechanical perturbation $\epsilon a(t)A$ is turned on, where $a(t)$ is a real analytic function with $a(0) = 0$,

$\epsilon > 0$, and $A = A^* \in B_0$. The *response* of an observable B to the driving potential $\epsilon a(t)A$ is defined to be

$$\begin{aligned} F^\lambda(t) &= \mathrm{tr}[B \otimes 1\, V_\lambda(t, 0)\, \rho_\beta \otimes v] \\ &= \mathrm{tr}[B\rho_\lambda(t)], \qquad \rho_\lambda(0) = \rho_\beta \end{aligned} \tag{16}$$

where $V_\lambda(t, 0)$ and $\rho_\lambda(t)$ are defined as in Section 2, with $H_t = H + \epsilon a(t)A$. The result of the last two sections is

$$\lim_{\lambda \to 0} \sup_{0 \leqslant t \leqslant t_0} |F^\lambda(t) - \mathrm{tr}[BW(t)Y(t)\rho_\beta]| = 0 \tag{17}$$

since $X_\lambda(t)\rho_\beta = \rho_\beta$. We emphasize that this result does not depend upon ϵ being small.

The basic assertion of the linear response theory is that for the behavior of the system close to equilibrium it is sufficient to study the response linear in the driving potential, i.e., to first order in ϵ. Therefore, the aim of the present section is to investigate $\mathrm{tr}[BW(t)Y(t)\rho_\beta]$ to first order in ϵ. We introduce explicitly the ϵ dependence as an additional argument, e.g., $W(t, \epsilon)$ is the solution of (11) with $H_t = H + \epsilon a(t)A$. Since $W(t, 0) = 1$, it follows that $Y(t, 0)$ is a quantum dynamical semigroup, whose generator we denote by L. If $E_n(\epsilon)$ are the spectral projections of $H + \epsilon A$ (analytically extended through the points of accidental degeneracies), $E_n(0) = E_n$, and if $e_n(\epsilon)$ are the corresponding eigenvalues, $e_n(0) = e_n$, then

$$\begin{aligned} L\rho = \sum_{\omega \in \mathrm{Sp}([H,.])} \sum_{i,j=1}^{N} \big(&-is_{ij}(\omega)[Q_j^*(\omega)Q_i(\omega), \rho] \\ &+ \hat{h}_{ij}(\omega)\{[Q_i(\omega)\rho, Q_j^*(\omega)] + [Q_i(\omega), \rho Q_j^*(\omega)]\}\big) \end{aligned} \tag{18}$$

$\hat{h}_{ij}$ is the Fourier transform of h_{ij}, s_{ij} is the Hilbert transform of h_{ij}, and

$$Q_j(\omega) = \sum_{e_m - e_n = \omega} E_n Q_j E_m$$

Note that L may be different from the operator called $L^\natural$ in Ref. 8 because of accidental degeneracies.

In the sequel certain invariance properties of the canonical equilibrium state of the system are used, which we therefore collect in the following lemma.

Lemma 3. Let

$$\rho_\beta(t, \epsilon) = e^{-\beta H_t}/\mathrm{tr}\, e^{-\beta H_t} \tag{19}$$

let

$$\begin{aligned} \bar{L}(t, \epsilon) &= W(t, \epsilon)L(t, \epsilon)^\natural W(t, \epsilon)^{-1} \\ &= \sum_n P_n(t, \epsilon)L(t, \epsilon)P_n(t, \epsilon) \end{aligned} \tag{20}$$

and let $U_t(s, \epsilon)$ be the unitary group on $\mathscr{B}_0$ generated by $Z(s, \epsilon) = -i[H + \epsilon a(s)A, \cdot]$. Then

$$\bar{L}(s, \epsilon)\rho_\beta(s, \epsilon) = 0 \tag{21}$$

$$U_t(s, \epsilon)\rho_\beta(s, \epsilon) = \rho_\beta(s, \epsilon) \tag{22}$$

Let $P_0(s, \epsilon)$ be the projection corresponding to the eigenvalue $\omega_0(s, \epsilon) \equiv 0$ of $Z(s, \epsilon)$. Then

$$P_0(s, \epsilon)\rho_\beta(s, \epsilon) = \rho_\beta(s, \epsilon), \qquad P_n(s, \epsilon)\rho_\beta(s, \epsilon) = 0 \tag{23}$$

for $n \neq 0$.

Proof. Both (21) and (22) are proved in Ref. 8; and (23) follows from the fact that $\rho_\beta(t, \epsilon)$ is an eigenvector of $Z(t, \epsilon)$ corresponding to the eigenvalue zero. ∎

We observe that

$$\begin{aligned}\frac{d}{dt} W(t, \epsilon)Y(t, \epsilon)f &= K(t, \epsilon)W(t, \epsilon)Y(t, \epsilon)f + W(t, \epsilon)L(t, \epsilon)^\natural Y(t, \epsilon)f \\ &= [K(t, \epsilon) + \bar{L}(t, \epsilon)]W(t, \epsilon)Y(t, \epsilon)f \end{aligned}\tag{24}$$

with $\bar{L}(t, \epsilon)$ defined in (20). Let $F_{BA}(t, \epsilon) = \operatorname{tr}[BW(t, \epsilon)Y(t, \epsilon)\rho_\beta]$. Then

$$\begin{aligned}&(1/\epsilon)\{\operatorname{tr}[BW(t, \epsilon)Y(t, \epsilon)\rho_\beta] - \operatorname{tr}[B\rho_\beta]\} \\ &\quad = \int_0^t ds \operatorname{tr}\{BY(t - s, 0)(1/\epsilon)[K(s, \epsilon) + \bar{L}(s, \epsilon) - L]W(s, \epsilon)Y(s, \epsilon)\rho_\beta\}\end{aligned}$$

Since $W(t, 0) = 1$ and $Y(t, 0)\rho_\beta = \rho_\beta$, the *linear response* is given by

$$F_{BA}^{\cdot}(t, 0) = \int_0^t ds \operatorname{tr}\{BY(t - s, 0)[K^{\cdot}(s, 0) + \bar{L}^{\cdot}(s, 0)]\rho_\beta\} \tag{25}$$

where the dot denotes the partial derivative with respect to ϵ.

Theorem 3. The linear response is

$$\begin{aligned}F_{BA}^{\cdot}(t, 0) = &\int_0^t ds\, a(t - s)\beta \operatorname{tr}\{[L^*B(s)](PA)\rho_\beta\} \\ &- a(t)\int_0^\beta d\alpha \operatorname{tr}\{Be^{-\alpha H}[(1 - P)A]e^{\alpha H}\rho_\beta\}\end{aligned}\tag{26}$$

with $B(t) = Y(t, 0)^*B = [\exp(L^*t)]B$ and $PA = P_0(t, 0)A = \sum_n E_nAE_n$.

Proof. From the proof of Lemma 1 we obtain $K(s, \epsilon) = \sum_n P_n'(s, \epsilon) P_n(s, \epsilon)$. Partial differentiation with respect to ϵ yields

$$K^{\cdot}(s, 0)\rho_\beta = \sum_n [P_n^{\cdot\prime}(s, 0)P_n(s, 0) + P_n'(s, 0)P_n^{\cdot}(s, 0)]\rho_\beta = P_0^{\cdot\prime}(s, 0)\rho_\beta$$

where we used Lemma 3 and $P_n'(s, 0) = 0$. A differentiation of (23) implies that

$$P_0^{\cdot}(s, 0)\rho_\beta + P\rho_\beta^{\cdot}(s, 0) = \rho_\beta^{\cdot}(s, 0)$$

We have

$$\rho_\beta^{\cdot}(s, 0) = -a(s)\int_0^\beta d\alpha\, e^{-\alpha H} A e^{\alpha H}\rho_\beta + \beta a(s)\rho_\beta \operatorname{tr}[A\rho_\beta] \tag{27}$$

Therefore

$$K^{\cdot}(s, 0)\rho_\beta = -a'(s)\int_0^\beta d\alpha\, e^{-\alpha H}[(1 - P)A]e^{\alpha H}\rho_\beta$$

By integration by parts, using $a(0) = 0$, we obtain

$$\begin{aligned}
&\int_0^t ds \operatorname{tr}[B(t - s)K^{\cdot}(s, 0)\rho_\beta] \\
&\quad = -a(t)\int_0^\beta d\alpha \operatorname{tr}\{Be^{-\alpha H}[(1 - P)A]e^{\alpha H}\rho_\beta\} \\
&\qquad + \int_0^t ds\, a(s)\int_0^\beta d\alpha \operatorname{tr}\{[L^* B(t - s)]e^{-\alpha H}[(P - 1)A]e^{\alpha H}\rho_\beta\}
\end{aligned} \tag{28}$$

A differentiation of (21) leads, using $\bar{L}(s, 0) = L$ and (27), to

$$\begin{aligned}
\bar{L}^{\cdot}(s, 0)\rho_\beta &= -L\rho_\beta^{\cdot}(s, 0) \\
&= -L\left\{-a(s)\int_0^\beta d\alpha\, e^{-\alpha H}Ae^{\alpha H}\rho_\beta + \beta a(s)\rho_\beta \operatorname{tr}[A\rho_\beta]\right\} \\
&= a(s)\int_0^\beta d\alpha\, Le^{-\alpha H}Ae^{\alpha H}\rho_\beta
\end{aligned}$$

since $L\rho_\beta = 0$. Adding (28) and $\int_0^t ds \operatorname{tr}[B(t - s)\bar{L}^{\cdot}(s, 0)\rho_\beta]$ yields (26). ∎

Equation (26) describes two effects. Since L^* commutes with P,[8] the driving force PA results in a response in PB, which is of the form familiar from linear response theory. $(1 - P)A$ produces an instantaneous response in $(1 - P)B$.

We note a few simple consequences of Theorem 3. Let $a(t) = a$ for $0 < t_0 \leqslant t$ and interpolate smoothly on $[0, t_0]$ between 0 and a. [Since $a(t)$

cannot be analytic under these assumptions, Theorem 3 does not apply. Nevertheless, we do not want to complicate the argument by choosing an approximating sequence of analytic functions.] Then

$$\lim_{t\to\infty} F_{BA}^{\cdot}(t,0) = \lim_{t\to\infty}\Big(a\beta\,\mathrm{tr}[B(t-t_0)(PA)\rho_\beta] - a\beta\,\mathrm{tr}[B(PA)\rho_\beta] + \int_{t-t_0}^{t} ds\, a(t-s)\,\mathrm{tr}\{[L^*B(s)](PA)\rho_\beta\} - a\int_0^\beta d\alpha\,\mathrm{tr}\{Be^{-\alpha H}[(1-P)A]e^{\alpha H}\rho_\beta\}\Big) \tag{29}$$

By assumption L^* has no purely imaginary eigenvalues, so $\mathrm{tr}\{[L^*B(t)](PA)\rho_\beta]$ decays exponentially fast. Therefore, the third term goes to zero. Furthermore, $\lim_{t\to\infty} B(t) = 1\,\mathrm{tr}[B\rho_\beta]$. Adding all terms in (29), we obtain

$$\lim_{t\to\infty} F_{BA}^{\cdot}(t,0) = a\left\{-\int_0^\beta d\alpha\,\mathrm{tr}[Be^{-\alpha H}Ae^{\alpha H}\rho_\beta] + \beta\,\mathrm{tr}[B\rho_\beta]\,\mathrm{tr}[A\rho_\beta]\right\} \tag{30}$$

which is the isothermal static (equilibrium) response.

For a periodic perturbation $(\sin\omega t)A$ we have two contributions. The second term in (26) gives a response proportional to $\sin\omega t$. The response from the first term is

$$\int_0^t ds\,(\sin\omega t\cos\omega s - \cos\omega t\sin\omega s)\beta \times \mathrm{tr}\{[L^*PB(s)]A\rho_\beta\} \equiv F_1^{\cdot}(t,0)$$

Therefore, after some initial time span, $F_1^{\cdot}(t,0)$ oscillates at the same frequency ω with a certain phase shift, i.e.,

$$\lim_{t\to\infty}[F_1^{\cdot}(t,0) - \mathrm{Im}\,\chi(\omega)e^{i\omega t}] = 0$$

with

$$\chi(\omega) = \int_0^\infty dt\, e^{-i\omega t}\Phi_{BA}(t) = -\mathrm{tr}\{[(L^* - i\omega)^{-1}L^*PB]A\rho_\beta\} \tag{31}$$

Here, $\Phi_{BA}(t) = \mathrm{tr}\{[L^*PB(t)]A\rho_\beta\}$ is the so-called response function obtained from an impulsive perturbation $a(t)\to\delta(t)$. It seems natural to define $\chi(\omega)$ as the generalized susceptibility (admittance) of the system. Then (31) agrees with the standard expression of linear response theory for the susceptibility, provided that the Hamiltonian dynamics $e^{itH}Be^{-itH}$ is replaced by $[\exp(L^*t)]PB$, corresponding to the time evolution of the open system.

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