Journal of Statistical Physics, Vol. 90, Nos. 3/4, 1998

Diagonalization of System plus Environment Hamiltonians

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Received July 8, 1997; final September 16, 1997

A new approach to dissipative quantum systems modeled by a system plus environment Hamiltonian is presented. Using a continuous sequence of infinitesimal unitary transformations, the small quantum system is decoupled from its thermodynamically large environment. Dissipation enters through the observation that system observables generically "decay" completely into a different structure when the Hamiltonian is transformed into diagonal form. The method is particularly suited for studying low-temperature properties. This is demonstrated explicitly for the super-Ohmic spin-boson model.

KEY WORDS: Dissipative quantum systems; flow equations; spin-boson model.

Dissipative behaviour in quantum physics can be modelled in a system plus bath framework.[1] The quantum system that one is interested in is described by a Hamiltonian H_S operating on the system Hilbert space $\mathscr{H}_S$, the thermodynamically large environment by some Hamiltonian H_B operating on $\mathscr{H}_B$. The full Hamiltonian H: $\mathscr{H}_S \otimes \mathscr{H}_B \to \mathscr{H}_S \otimes \mathscr{H}_B$ of system plus bath is obtained by coupling $\mathscr{H}_S$ and $\mathscr{H}_B$ with some interaction H_{SB}

$$H = H_S \otimes \mathbb{1}_B + \mathbb{1}_S \otimes H_B + H_{SB} \tag{1}$$

Most theoretical work starts off by tracing out the bath degrees of freedom and then using suitable approximation schemes for the time evolution of

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0022-4715/98/0200-0889$15.00/0 © 1998 Plenum Publishing Corporation

the reduced density matrix of the small quantum system (for a review see, e.g., ref. 2). In this letter we present an alternative approach that aims at decoupling system and bath with a unitary transformation U

$$UHU^{\dagger} = \tilde{H}_S \otimes \mathbb{1}_B + \mathbb{1}_S \otimes \tilde{H}_B \tag{2}$$

Here $\tilde{H}_S$ and $\tilde{H}_B$ are modified system and bath Hamiltonians. By carrying out this programme in the manner described below this approach is particularly suited for studying low-temperature properties of dissipative quantum systems, thereby being complementary to most other approximation schemes.

For a finite system a transformation U as in (2) will always exist. Let us already mention, however, that a subtle problem can occur in the thermodynamic limit regarding the interpretation of the eigenstates of $\tilde{H}_S \otimes \mathbb{1}_B$. We postpone this point until later when we discuss correlation functions.

As a specific example we demonstrate these ideas for the spin-boson model

$$H = -\frac{\Delta}{2}\sigma_x + \sum_k \omega_k b_k^{\dagger} b_k + \frac{1}{2}\sigma_z \sum_k \lambda_k (b_k^{\dagger} + b_k) \tag{3}$$

describing a two-level system coupled to a bath modelled by harmonic oscillators. The standard approach to this problem is the "Non-Interacting Blip Approximation" (NIBA) for the effective action obtained after integrating out the bath degrees of freedom.[3] In our approach we find low-temperature equilibrium correlation functions of the tunneling particle that combine NIBA-results at intermediate time scales with the correct long-time behaviour where the simple NIBA fails.[2] The universal Wilson ratio for a super-Ohmic bath put forward in ref. 4 is also obtained.

Extension of our scheme to other dissipative quantum systems is straightforward under the basic assumption that H_S has a non-degenerate ground state separated by a finite gap from its excited states. More technical details of our method can be found in ref. 5. New results in this letter are in particular the calculation of impurity contributions to the specific heat and of universal Wilson ratios that were still open problems in ref. 5.

Two obvious questions arise with respect to the programme (1)–(2). Where is dissipation in Eq. (2) as exchange of energy between system and bath is no longer possible? And how can one find a unitary transformation U that fulfills the required task?

We first discuss the second point. The decoupling of system and bath is achieved by a method of infinitesimal unitary transformations ("flow

equations") introduced by Wegner in ref. 6.[3] A suitable antihermitean generator $\eta(\ell) = -\eta(\ell)^\dagger$ is chosen and the initial-value problem

$$\frac{dH(\ell)}{d\ell} = [\eta(\ell), H(\ell)], \qquad H(\ell = 0) = H \tag{4}$$

solved. The parameter ℓ has dimension $(\text{Energy})^{-2}$. Equation (4) generates a one-parameter family of unitarily equivalent Hamiltonians $H(\ell)$. In the limit $\ell \to \infty$ one attempts to obtain a Hamiltonian $H(\ell = \infty)$ of the simple structure (2). The choice of $\eta(\ell)$ is inspired by renormalization theory: Initially for small ℓ matrix elements corresponding to large energy differences between system and bath are decoupled, for large ℓ one deals with the nearly resonant modes. The fundamental problem of (4) is that higher and higher order interactions are successively generated. So a further condition for $\eta(\ell)$ is that the number of additional terms should be small. Finally $\eta(\ell)$ must commute with symmetry operators of the initial problem, so that $H(\ell)$ has the same symmetries as $H(0)$. These conditions essentially fix a unique structure of $\eta(\ell)$

$$\eta = \imath\sigma_y \sum_k \eta_k^{(y)}(b_k + b_k^\dagger) + \sigma_z \sum_k \eta_k^{(z)}(b_k - b_k^\dagger) + \sum_{k,q} \eta_{k,q} :(b_k + b_k^\dagger)(b_q - b_q^\dagger): \tag{5}$$

with

$$\begin{aligned} \eta_k^{(y)} &= -\frac{1}{2}\lambda_k \Delta \frac{\omega_k - \Delta}{\omega_k + \Delta}, \qquad \eta_k^{(z)} = \frac{\omega_k}{\Delta}\eta_k^{(y)}, \\ \eta_{k,q} &= \frac{\lambda_k \lambda_q \Delta \omega_q}{2(\omega_k^2 - \omega_q^2)} \tanh\frac{\beta\Delta}{2}\left(\frac{\omega_k - \Delta}{\omega_k + \Delta} + \frac{\omega_q - \Delta}{\omega_q + \Delta}\right) \end{aligned} \tag{6}$$

All parameters in (6) depend on ℓ and normal-ordering with respect to the non interacting ground state has been introduced. For the construction of generators η in a general setting see refs. 5, 6. The only new interaction terms generated in the first application of (4) is $:\sigma_x(b_k \pm b_k^\dagger)(b_{k'} \pm b_{k'}^\dagger):$.

Due to the flow the spectral function $J(\omega) = \sum_k \lambda_k^2 \delta(\omega - \omega_k)$ describing the coupling of system and bath becomes ℓ-dependent too, $J(\omega, \ell) = \sum_k \lambda_k(\ell)^2 \delta(\omega - \omega_k)$, $J(\omega, \ell = 0) = J(\omega)$. We end up with the following set of differential equations for the couplings in the Hamiltonian by comparing the lhs and rhs of (4)

[3] Similar ideas have recently also been introduced in high-energy physics by Glazek and Wilson[7] for the investigation of bound states in light-front QCD.

$$\frac{d\Delta}{d\ell} = -\Delta \int d\omega\, J(\omega, \ell)\, \frac{\omega - \Delta}{\omega + \Delta} \coth \frac{\beta\omega}{2} \tag{7}$$

$$\frac{\partial J(\omega, \ell)}{\partial \ell} = -2(\omega - \Delta)^2 J(\omega, \ell) + 2\Delta \tanh \frac{\beta\Delta}{2} J(\omega, \ell) \times \int d\omega' \frac{\omega' J(\omega', \ell)}{\omega^2 - \omega'^2} \left(\frac{\omega - \Delta}{\omega + \Delta} + \frac{\omega' - \Delta}{\omega' + \Delta} \right) \tag{8}$$

and a differential equation for an uninteresting additive term in (3) corresponding to the ground state energy. The differential equation for the higher normal-ordered interaction term $:\sigma_x(b_k \pm b_k^\dagger)(b_{k'} \pm b_{k'}^\dagger):$ is subsequently neglected. This approximation can be systematically improved by taking such higher-order interactions that are also of higher order in the small parameters λ_k into account one after the other in the hierarchy of differential equations. However, already the above approximation leads to a very satisfactory description as will be shown.

As required large energy differences are first decoupled in (8) and small energy differences later. For $\ell \to \infty$ the coupling $J(\omega, \ell)$ vanishes for all ω, in general exponentially and for $\omega = \Delta(\ell = \infty)$ algebraically. Within the above approximations one ends up with a system Hamiltonian $\tilde{H}_S = -1/2\, \Delta_r \sigma_x$ that is decoupled from the environment. Here $\Delta_r = \Delta(\ell = \infty)$ is the renormalized tunneling matrix element. By either numerical solution of the differential equations or analytical approximations one finds $\Delta_r = c\, \Delta_0 \exp(-(\omega_c/K)^{s-1}/(2s-2))$ for a super-Ohmic bath $J(\omega) = K^{1-s}\omega^s \Theta(\omega_c - \omega)$ with $s > 1$. Here $\Delta_0 = \Delta(\ell = 0)$, c is a constant of order 1, ω_c some high-energy cutoff and K the coupling constant. Δ_r defines the low-energy scale of the problem in agreement with other methods (see, e.g., ref. 3).

For small $\ell \ll \Delta_r^{-2}$ the above procedure is equivalent to Anderson's "poor man's" scaling[8] with a smooth cutoff, except that the high-energy states are not removed by integrating them out but by decoupling them using unitary transformations (see Fig. 1). By explicitly finding this unitary transformation no information about the removed states is lost but contained in the unitary transformation itself.[4] Scaling approaches have to stop when the effective band edge becomes of order the low-energy scale of the problem due to divergencies in the renormalization group equations. The flow equations can be integrated further since with our choice of $\eta(\ell)$ decoupling is with respect to energy differences and does not only take place at the effective band edge.

[4] In principle it is possible to reconstruct the full unitary transformation U in (2) by evaluating ℓ-ordered products of $\eta(\ell)$, but the differential approach is more appropriate.

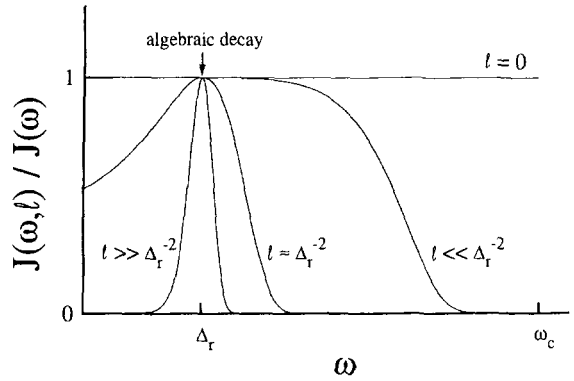

Fig. 1. Schematic behaviour of the effective spectral function $J(\omega, \ell)$ for various regimes of the flow equations.

In the region $\ell \gtrsim \Delta_r^{-2}$ that remains unreachable in the "poor man's" approach new features appear that are hidden for smaller ℓ. First of all the flow of the parameters in the Hamiltonian becomes negligible and has a universal algebraic ℓ-dependence $\ell^{-1/2}$. In contrast the transformation of the system observables turns out to be essential in this regime. In the crossover region $\ell \approx \Delta_r^{-2}$ both flow of parameters and system observables are important.

As a specific example for this scenario we discuss the symmetrized equilibrium correlation function describing the tunneling particle $C(t) = \frac{1}{2}\langle\{\sigma_z(t), \sigma_z(0)\}\rangle$. In order to use the trivial time evolution with respect to the Hamiltonian $H(\ell = \infty)$ we have to transform the observable σ_z as well

$$\frac{d\sigma_z(\ell)}{d\ell} = [\eta(\ell), \sigma_z(\ell)], \qquad \sigma_z(\ell = 0) = \sigma_z \tag{9}$$

These differential equations cannot be solved in closed form and we have to make an ansatz for the transformation of $\sigma_z(\ell)$

$$\sigma_z(\ell) = h(l)\,\sigma_z + \sigma_x \sum_k \chi_k(\ell)(b_k + b_k^\dagger) \tag{10}$$

where higher normal-ordered terms are neglected. One obtains the following differential equations

$$\begin{aligned} \frac{dh}{d\ell} &= -\Delta \sum_k \lambda_k \chi_k \frac{\omega_k - \Delta}{\omega_k + \Delta} \coth \frac{\beta\omega_k}{2} \\ \frac{d\chi_k}{d\ell} &= \Delta h \lambda_k \frac{\omega_k - \Delta}{\omega_k + \Delta} + \Delta\lambda_k \tanh \frac{\beta\Delta}{2} \sum_q \frac{\chi_q \lambda_q \omega_q}{\omega_k^2 - \omega_q^2} \left(\frac{\omega_k - \Delta}{\omega_k + \Delta} + \frac{\omega_q - \Delta}{\omega_q + \Delta} \right) \end{aligned} \tag{11}$$

One can prove $h(\ell=\infty)=0$ if Δ_r lies in the support of $J(\omega)$. Therefore $\sigma_z(\ell)$ in (10) decays completely under the sequence of unitary transformations, which is essential to see dissipative behaviour with a Hamiltonian like (2). In general one can show for a system observable $O\otimes \mathbb{1}_B$ that does not commute with the algebra spanned by $[H_S\otimes \mathbb{1}_B, H_{SB}]$: If some excitation energy from the ground state of $\tilde{H}_S$ lies in the support of the spectral function then the observable decays completely when transforming from (1) to (2) in the sense that no such term of structure $O\otimes \mathbb{1}_B$ survives.[5] This result also holds in the zero-temperature limit.

In fact these properties of the observables are related to the problem mentioned below Eq. (2): The right hand side of Eq. (2) can contain discrete eigenstates embedded in the continuum generated by $\tilde{H}_B$ in the thermodynamic limit. This is known to be wrong.[9] In order to resolve this problem one has to investigate the eigenstate corresponding to the embedded eigenvalue when it is transformed back to $\ell=0$. One observes that this eigenstate decays completely into a sum of bath states. The weights of these bath states vanish in the limit $\ell\to 0$ for a thermodynamically large system. Therefore this state has to be excluded from the space of physical states. We have seen above that this unphysical state does not show up in the correlation functions calculated using the transformed operators anyway, so we can ignore this point in the sequel. In general one has to be cautious since the thermodynamic limit and the limit $\ell\to\infty$ do not generally commute.

The one-sided Fourier transform $C(\omega)$ of the correlation function $C(t)=\int_0^\infty d\omega\, C(\omega)\cos(\omega t)$ can be expressed as $C(\omega)=\sum_k \chi_k^2(\infty)\times \coth(\beta\omega_k/2)\,\delta(\omega-\omega_k)$ and the $\chi_k(\infty)$ have to be found numerically. This is simplified by the following observation. For $\ell\to\infty$ the remaining spectral function $J(\omega,\ell)$ is strongly peaked around Δ_r (Fig. 1). In this limit the exactly solved dissipative harmonic oscillator[10]

$$H=\Delta b^\dagger b+\sum_k \omega_k b_k^\dagger b_k+(b+b^\dagger)\sum_k \lambda_k(b_k+b_k^\dagger) \tag{12}$$

becomes equivalent to a two-state system as the mean occupation number $\langle b^\dagger b\rangle$ of the dissipative harmonic oscillator at zero temperature goes to zero with the width of the spectral function. The corresponding set of differential equations (7, 8, 11, 12) for the dissipative harmonic oscillator can be solved in closed form.[5] This solution is exact as no higher-order terms in the Hamiltonian or the transformation of observables appear. Formally this can be seen by introducing functions $S_0(z,\ell)=\sum_k \omega_k\lambda_k^2/(z-\omega_k^2)$, $S_1(z,\ell)=\sum_k \sqrt{\omega_k\Delta}\,\chi_k\lambda_k/(z-\omega_k^2)$, $S_2(z,\ell)=\sum_k \chi_k^2/(z-\omega_k^2)$ and by showing

$$S_2(z,\infty)=S_2(z,\ell_0)-\frac{(h(\ell_0)+S_1(z,\ell_0))^2}{\Delta(\ell_0)^2-z+\Delta(\ell_0)\,S_0(z,\ell_0)}+O(\ell_0^{-1}) \tag{13}$$

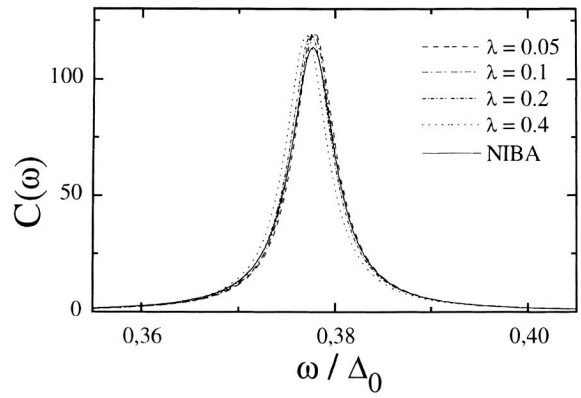

Fig. 2. Exemplary correlation function for a super-Ohmic bath ($s=2$, $K=40$, $\omega_c=80$). The different curves are obtained by using Eq. (13) for various values of $\ell_0=(2\lambda\Delta_r)^{-2}$. The scale is set by $\Delta_0=1$. For comparison the NIBA-curve is also shown. The maximum of the NIBA-curve is slightly shifted with respect to the flow equations and has been suitably rescaled in order to identify the peaks.

For the dissipative harmonic oscillator (13) holds exactly without the term $O(\ell_0^{-1})$. Numerically the correlation function $C(\omega)=-2\omega/\pi\,\mathscr{I}\times S_2(\omega^2-i0_+,\infty)$ has been obtained by integrating the flow equations up to some $\ell_0=(2\lambda\Delta_r)^{-2}$, $\lambda\ll 1$, thereby obtaining $S_2(z,\ell_0)$ and then adding the second term from (13) that describes a dissipative harmonic oscillator with the spectral function $J(\omega,\ell_0)$. Therefore the resolution of the peak in $C(\omega)$ for $\omega=\Delta_r$ is not limited by $\ell_0^{-1/2}$. By using the analogy with the dissipative harmonic oscillator we are restricted to low temperatures $T\ll\Delta_r$.

Some zero-temperature correlation functions obtained in this manner are shown in Fig. 2. The final results vary very little with λ as long as $\lambda\lesssim 0.5$. This gives a posteriori justification of our approximations. For $\ell\ll\Delta_r^{-2}$ the neglected terms are irrelevant in the usual scaling sense, for $\ell\gg\Delta_r^{-2}$ our equations are closed due to the analogy with the dissipative harmonic oscillator. As the final results for super-Ohmic baths do not depend on where these two parts are matched in the crossover region, it is reasonable to argue that the approximations are also good for $\ell\approx\Delta_r^{-2}$.[5]

The correlation functions obtained for such parameters are in good agreement with the NIBA for intermediate time scales (Fig. 2). That is for $\omega\approx\Delta_r$ the curves are well-described by a Lorentzian with a peak at $\omega=\Delta_r$

[5] For an Ohmic bath $J(\omega)\propto\omega$ with intermediate and strong coupling the final result for $C(\omega)$ depends on λ. This is due to our simple choice of $\eta_{k,q}$ that generates an IR-problem for Ohmic baths.[15] Hence we restrict ourselves to super-Ohmic baths in this letter.

Table I. Representative Results from the Numerical Solution of the Flow Equations for Super-Ohmic Baths $J(\omega) = K^{1-s}\omega^s \Theta(\omega_c - \omega)$[a]

s	ω_c	K	χ_0	$\left[\frac{C(\omega)}{J(\omega)}\right]_{\omega\to 0}$	$\left[\frac{C(\omega)}{(2\chi_0)^2 J(\omega)}\right]_{\omega\to 0}$	R_s	$R_s^{(\text{theor})}$
2	80	40	1.31	7.12	1.04	0.370	0.361
2	160	80	1.34	7.24	1.01	0.182	0.180
2	320	160	1.35	7.31	1.00	0.090	0.090
2	80	20	3.40	47.4	1.03	0.734	0.721
2	160	40	3.54	50.6	1.01	0.363	0.361
2	320	80	3.62	52.5	1.00	0.180	0.180
2	80	10	22.6	2.05×10^3	1.01	1.43	1.44
2	160	20	24.7	2.45×10^3	1.00	0.718	0.721
2	320	40	25.9	2.69×10^3	1.00	0.359	0.361
3	20	10	1.26	6.68	1.05	0.786	0.779
3	40	20	1.31	6.93	1.01	0.194	0.195
3	60	30	1.33	7.05	1.00	0.0858	0.0866
3	10	3.33	3.52	52.4	1.06	7.39	7.03
3	20	6.67	3.71	55.8	1.01	1.78	1.75
3	30	10	3.98	63.8	1.01	0.783	0.779

[a] The scale is set by $\Delta_0 = 1$. $R_s^{(\text{theor})}$ is the Wilson ratio from (18). Numerical errors for the Shiba and the Wilson ratio are estimated as 2%.

and half width $\pi/2\, J(\Delta_r)$.[6] For long times the NIBA fails as it predicts an exponential decay at $T = 0$,[3] whereas the long-time behaviour is known to be determined by the low-frequency behaviour of the spectral function. This is made explicit in the Shiba-relation[11] generalized to super-Ohmic baths in ref. 4 (note our normalization $\int_0^\infty C(\omega)\, d\omega = 1$)

$$\lim_{\omega\to 0} \frac{C(\omega)}{(2\chi_0)^2 J(\omega)} = 1 \tag{14}$$

with the static susceptibility χ_0. χ_0 can be extracted with a Kramer's–Kronig relation and a fluctuation-dissipation theorem $\chi_0 = 1/2 \int_0^\infty C(\omega)/\omega\, d\omega$. The numerical solution of the flow equations is in excellent agreement with the Shiba-relation (Table I). One observes only small deviations that disappear in the limit $\omega_c \gg \Delta_0$, $\Delta_r = \text{const.}$ (or $\omega_c/K = \text{const.}$). For an Ohmic bath the Shiba-relation was recently verified numerically by Costi and Kieffer using Wilson's numerical renormalization group method.[12]

[6] This can also be shown analytically by an approximate solution of the set of differential equations, see ref. 5.

Another interesting low-energy property is the impurity contribution to the specific heat $c_i(T)$. This quantity is trivial to obtain from a Hamiltonian like (2). But it follows from the difference of two extensive quantities and it becomes necessary to discuss the flow equations for the bath energies too. That could be ignored before since the couplings λ_k scale with $1/\sqrt{N}$ where N is the number of bath modes. One finds

$$\frac{d\omega_k}{d\ell} = \Delta\, \lambda_k^2\, \frac{\omega_k - \Delta}{\omega_k + \Delta} \tag{15}$$

and the impurity contribution to the internal energy for $T \ll \Delta_r$ is simply

$$E_i = \sum_k \frac{\omega_k(\infty)}{e^{\beta\omega_k(\infty)} - 1} - \sum_k \frac{\omega_k(0)}{e^{\beta\omega_k(0)} - 1} \tag{16}$$

For super-Ohmic baths $J(\omega) \propto \omega^s$ for small ω, $s > 1$, one derives the following expression for the impurity contribution to the specific heat $c_i = dE_i/dT$

$$c_i = sT^s \Gamma(s+2)\, \zeta(s+1) \int_0^\infty d\ell\, \Delta(\ell)\, g(\ell) \tag{17}$$

with $g(\ell)$ defined from $J(\omega, \ell) = g(\ell)\, \omega^s + O(\omega^{s+1})$. In particular the impurity contribution to the specific heat is not Schottky-like but scales as T^s. A sensitive test is provided by the Wilson ratio $R_s = \lim_{T \to 0} c_i(T)/(\chi_0\, T^s)$ also generalized to super-Ohmic baths in ref. 4

$$R_s = s\Gamma(s+2)\, \zeta(s+1) \lim_{x \to 0} \frac{J(x)}{x^s} \tag{18}$$

Wilson ratios obtained from the numerical solution of the flow equations can be found in Table I. Agreement with (18) is excellent in the limit $\omega_c \gg \Delta_0$, $\Delta_r = \text{const}$.

Summing up, we have applied a new approximation method based on infinitesimal unitary transformations[6] to the spin-boson model. The method is an extension of "poor man's" scaling[8] as it allows to decouple modes below the low-energy scale of the model. Instead of renormalization group equations with respect to the effective band width we have differential equations with respect to energy differences parametrized by ℓ. An essential new feature as compared to the scaling approach is the transformation of the observables once the decoupling has reached the low-energy scale. Thereby we have successfully matched formal solutions[4] yielding the

Shiba-relation and universal Wilson ratios with the well-established NIBA at intermediate energies in one consistent scheme.

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Communicated by J. L. Lebowitz