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Sufficient conditions for positivity of non-Markovian master equations with Hermitian generators

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Abstract
We use basic physical motivations to develop sufficient conditions for positive semidefiniteness of the reduced density matrix for generalized non-Markovian integrodifferential Lindblad–Kossakowski master equations with Hermitian generators. We show that it is sufficient for the memory function to be the Fourier transform of a real positive symmetric frequency density function with certain properties. These requirements are physically motivated, and are more general and more easily checked than previously stated sufficient conditions. We also explore the decoherence dynamics numerically for some simple models using the Hadamard representation of the propagator. We show that the sufficient conditions are not necessary conditions. We also show that models exist in which the long time limit is in part determined by non-Markovian effects.

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1. Introduction

Recent interest in controlling quantum interference [1] for applications in nano-technology [2], quantum computing [3] and cryptography, and control of molecular processes [4] has motivated efforts to develop generalized master equations [5–15] for the evolution of open systems. Condensed phase environments are frequently encountered in such applications, and since such environments may be chaotic [16–18], the exact master equations developed for environments consisting of the non-interacting modes of the radiation field [19–24] are generally inapplicable. In addition, the exact general Nakajima–Zwanzig [25] master equation is inapplicable because it is impossible to numerically evaluate the memory kernel.

Approximate but very useful master equation theories have been developed for the special case of Markovian evolutions [26]. These Lindblad–Kossakowski type master equations preserve the positivity of the system reduced density matrix as well as the complete positivity

[26]. Recently there have been many attempts to generalize these equations to the non-Markovian regime [5–15] appropriate for complex environments.

In a few cases attempts have been made to establish sufficient conditions under which integrodifferential generalizations of the Lindblad–Kossakowski [26] equations preserve positivity [11, 14, 15] and complete positivity [6]. The sufficient conditions for positivity are at least as important as those for complete positivity because they are expected to be weaker, and many useful but approximate theories may violate complete positivity. Existing sufficient conditions for positivity are rather complicated and their introduction was motivated more by mathematical considerations than by physical constraints. Thus it would be useful to develop constraints which are motivated directly from features of the dynamics of the reduced density matrix. In addition, such an analysis could be useful if the simplest mathematical arguments are used and these focus on a physically interesting object. We will show that most of the analysis can be focused on the Hadamard representation of the dissipative propagator.

A second motivation for developing simple and general sufficient conditions for positivity is to, in some degree, counter the impression created by [15] that negativity is a serious problem. While the authors correctly demonstrate that a non-Markovian master equation with a non-Hermitian generator and memory function $K(t) \propto e^{-\gamma t}$ violates positivity, their 'warning against the use of approximate methods with memory' is far too general. It is well known that Lindblad–Kossakowski equations with non-Hermitian generators can be transformed into related Lindblad–Kossakowski equations with Hermitian generators. The result of [15] merely means that generalizations should be based on master equations with Hermitian generators.

Finally, it is important to realize that such non-Markovian master equations, which are of integrodifferential form, can now be readily solved numerically [27]. Thus the Markov approximation is no longer a practical necessity.

In this paper we establish the most general sufficient conditions for positive semidefinite reduced dynamics yet developed. We show that the memory function should be the Fourier transform of a real positive symmetric frequency density function with certain properties. This is more general than previous prescriptions, it is simpler to verify in practice and makes sense physically since the frequency density function in many cases has a physical meaning [11, 12, 24].

In section 2 we derive the sufficient conditions. In section 3 we calculate the eigenvalues of the Hadamard representation of the propagator for a number of different models for the frequency distribution function. We show that the sufficient conditions are not necessary conditions. We also show that in some cases the long time limit is affected by the memory function, meaning that the equilibrium density is determined by non-Markovian effects.

2. Sufficient conditions for positivity

Consider a non-Markovian master equation, with a Hermitian generator $\hat{q}$ and a real memory function $K(t)$, of the generalized Lindblad–Kossakowski form [26]

$$\frac{\mathrm{d}\hat{\rho}(t)}{\mathrm{d}t} = \int_0^t \mathrm{d}t'\, K(t-t')[2\hat{q}\hat{\rho}(t')\hat{q} - \hat{q}^2\hat{\rho}(t') - \hat{\rho}(t')\hat{q}^2]. \tag{1}$$

For simplicity we also assume that the eigenbasis of $\hat{q}$ is complete, i.e. $\hat{q}|q\rangle = q|q\rangle$ and $\sum_q |q\rangle\langle q| = 1$. This being the case we can represent $\hat{\rho}(t)$ by its matrix elements in this basis. It then follows, given $\rho_{q,q'}(t) = \langle q|\hat{\rho}(t)|q'\rangle$, that

$$\frac{\mathrm{d}\rho_{q,q'}(t)}{\mathrm{d}t} = -(q-q')^2 \int_0^t \mathrm{d}t'\, K(t-t')\rho_{q,q'}(t') \tag{2}$$

from which it immediately follows that $\rho_{q,q}(t) = \rho_{q,q}(0)$.

We assume that the initial density is positive semidefinite so that $\rho_{q,q}(0) \geqslant 0$ and $|\rho_{q,q'}(0)|^2 \leqslant \rho_{q,q}(0)\rho_{q',q'}(0)$.

Differentiation of $|\rho_{q,q'}(t)|^2$, using equation (2), yields

$$\frac{\mathrm{d}|\rho_{q,q'}(t)|^2}{dt} = -(q-q')^2 \int_0^t \mathrm{d}t' K(t-t')[\rho^*_{q,q'}(t')\rho_{q,q'}(t) + \rho^*_{q,q'}(t)\rho_{q,q'}(t')] \tag{3}$$

and integration of equation (3) then gives

$$|\rho_{q,q'}(t)|^2 - |\rho_{q,q'}(0)|^2 = -(q-q')^2 \int_0^t \mathrm{d}t' \int_0^{t'} \mathrm{d}t''\, K(t'-t'') \times [\rho^*_{q,q'}(t'')\rho_{q,q'}(t') + \rho^*_{q,q'}(t')\rho_{q,q'}(t'')]. \tag{4}$$

We wish to determine whether the right-hand side is always negative as would be expected for a decoherence process.

The exact memory kernel in the Nakajima–Zwanzig master equation [25] is time symmetric because the Liouville operator L is unitarily equivalent to $-L$. Thus the memory function in approximate master equations should inherit this symmetry and so $K(t) = K(-t)$, and we can simplify equation (4) to the form

$$|\rho_{q,q'}(t)|^2 - |\rho_{q,q'}(0)|^2 = -(q-q')^2 \int_0^t \mathrm{d}t' \int_0^t \mathrm{d}t''\, K(t'-t'')\rho^*_{q,q'}(t'')\rho_{q,q'}(t'). \tag{5}$$

However, the sign of the right-hand side is still undetermined.

In many exact [24] and approximate [11, 12] theories the memory function is the Fourier transform of a frequency density function. So suppose additionally that $K(t)$ is the Fourier Transform of an integrable positive real symmetric density function $p(\omega)$, i.e. $K(t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \mathrm{d}\omega\, p(\omega)\, \mathrm{e}^{-\mathrm{i}\omega t}$. In many cases one might instead have $K(t) = \sqrt{\frac{2}{\pi}} \int_0^{\infty} \mathrm{d}\omega\, p(\omega) \cos \omega t$, but defining $p(-\omega) = p(\omega)$ then $K(t)$ can be rewritten in the previous form.

With this form for $K(t)$ we may conclude that

$$|\rho_{q,q'}(t)|^2 - |\rho_{q,q'}(0)|^2 = -(q-q')^2 \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \mathrm{d}\omega\, p(\omega) \left| \int_0^t \mathrm{d}t'\, \rho_{q,q'}(t')\, \mathrm{e}^{-\mathrm{i}\omega t'} \right|^2. \tag{6}$$

Here the right-hand side is negative and so we know that $|\rho_{q,q'}(t)|^2 - |\rho_{q,q'}(0)|^2 \leqslant 0$. (Note that $p(\omega)$ is not necessarily normalized.)

Assuming that $\hat{\rho}(0)$ is positive semidefinite it follows that $|\rho_{q,q'}(0)|^2 \leqslant \rho_{q,q}(0)\rho_{q',q'}(0)$ (i.e. this is a necessary condition for non-negativity). Putting this together with our prior result and the fact that the diagonal matrix elements are stationary then implies that $|\rho_{q,q'}(t)|^2 \leqslant |\rho_{q,q'}(0)|^2 \leqslant \rho_{q,q}(0)\rho_{q',q'}(0) = \rho_{q,q}(t)\rho_{q',q'}(t)$. Now since $\rho(0)$ is positive semidefinite $\rho_{q,q}(0) \geqslant 0$, and so $\rho_{q,q}(t) \geqslant 0$. Thus, the time evolved density satisfies the same two necessary conditions for positivity that the initial density does.

Indeed, it now follows that the eigenvalues of the matrix

$$\begin{pmatrix} \rho_{q,q}(t) & \rho_{q,q'}(t) \\ \rho_{q',q}(t) & \rho_{q',q'}(t) \end{pmatrix},$$

namely

$$\tfrac{1}{2}[\rho_{q,q}(t) + \rho_{q',q'}(t) \pm \sqrt{(\rho_{q,q}(t) + \rho_{q',q'}(t))^2 - 4(\rho_{q,q}(t)\rho_{q',q'}(t) - |\rho_{q,q'}(t)|^2)}] \tag{7}$$

are both non-negative.

Thus, if a generator only has two eigenvalues then the sufficient condition for positivity is that $p(\omega)$ is real, positive and symmetric.

2.1. Hadamard representation

In the event that the generator has more than two eigenvalues the sufficient condition is still to be determined. In this case we define an operator $\hat{U}(t)$ via

$$\hat{\rho}(t) = \hat{U}(t) \circ \hat{\rho}(0) \tag{8}$$

where $\circ$ denotes the Hadamard product (i.e. $\rho_{q,q'}(t) = U_{q,q'}(t)\rho_{q,q'}(0)$) and invoke a standard theorem [30] which states that $\hat{\rho}(t)$ will be positive semidefinite if $\hat{U}(t)$ and $\hat{\rho}(0)$ are positive semidefinite. We will assume that $\hat{\rho}(0)$ is positive semidefinite and so we need to determine under what conditions $\hat{U}(t)$ is positive semidefinite.

We deduce from equation (2) and the definition of $\hat{U}(t)$ that

$$\frac{\mathrm{d}U_{q,q'}(t)}{\mathrm{d}t} = -(q-q')^2 \int_0^t \mathrm{d}t'\, K(t-t')U_{q,q'}(t') \tag{9}$$

with $U_{q,q'}(0) = 1$. One can then show using Laplace transform techniques that the Fourier transform $U_{q,q'}(\omega)$ of $U_{q,q'}(t)$ takes the form

$$U_{q,q'}(\omega) = \sqrt{\frac{2}{\pi}} \mathrm{Re} \frac{1}{-\mathrm{i}\omega + (q-q')^2 \tilde{K}(-\mathrm{i}\omega)} \tag{10}$$

where $\tilde{K}(z)$ is the Laplace transform of $K(t)$. With a bit of manipulation and the identity $1/(x+\mathrm{i}\epsilon) = \mathcal{P}(1/x) - \mathrm{i}\pi\delta(x)$ one can show that

$$\tilde{K}(-\mathrm{i}\omega) = \sqrt{\frac{\pi}{2}}[p(\omega) + \mathrm{i}\Delta(\omega)] \tag{11}$$

where

$$\Delta(\omega) = \frac{1}{\pi}\int_0^\infty \mathrm{d}x \frac{p(x-\omega) - p(x+\omega)}{x}. \tag{12}$$

Unfortunately, $\Delta(\omega)$ does not exist for every model of interest but it does exist for a very wide range of densities and so this limitation is not fatal.

It then follows that

$$U_{q,q'}(t) = \frac{1}{2}\int_{-\infty}^{\infty} \mathrm{d}\omega \frac{(q-q')^2 p(\omega)\,\mathrm{e}^{-\mathrm{i}\omega t}}{\left[\omega - \sqrt{\frac{\pi}{2}}(q-q')^2\Delta(\omega)\right]^2 + \frac{\pi}{2}(q-q')^4 p(\omega)^2}. \tag{13}$$

This formula can be viewed as a Hadamard representation of the dissipative propagator. Unfortunately, it is not directly useful for our purposes since any sufficient condition for positivity derived from this formula would depend on the spectrum of $\hat{q}$.

2.2. Frequency representation

Inserting a delta function in equation (13) and using the identity $\delta(x - (q-q')) = \frac{1}{2\pi}\int_{-\infty}^{\infty} \mathrm{d}\Omega\, \mathrm{e}^{\mathrm{i}(x-q+q')\Omega}$ it then follows that

$$U_{q,q'}(t) = \int_{-\infty}^{\infty} \mathrm{d}x \delta(x-(q-q'))\frac{1}{2}\int_{-\infty}^{\infty} \mathrm{d}\omega \frac{x^2 p(\omega)\,\mathrm{e}^{-\mathrm{i}\omega t}}{\left[\omega - \sqrt{\frac{\pi}{2}}x^2\Delta(\omega)\right]^2 + \frac{\pi}{2}x^4 p(\omega)^2} \tag{14}$$

$$= \int_{-\infty}^{\infty} \mathrm{d}x \frac{1}{2\pi}\int_{-\infty}^{\infty} \mathrm{d}\Omega\, \mathrm{e}^{\mathrm{i}(x-q+q')\Omega}\frac{1}{2}\int_{-\infty}^{\infty} \mathrm{d}\omega \frac{x^2 p(\omega)\,\mathrm{e}^{-\mathrm{i}\omega t}}{\left[\omega - \sqrt{\frac{\pi}{2}}x^2\Delta(\omega)\right]^2 + \frac{\pi}{2}x^4 p(\omega)^2} \tag{15}$$

$$= \frac{1}{2\pi}\int_{-\infty}^{\infty} \mathrm{d}\Omega\, \mathrm{e}^{-\mathrm{i}(q-q')\Omega} W(\Omega, t) \tag{16}$$

where

$$W(\Omega,t)=\int_{-\infty}^{\infty}\mathrm{d}\omega V(\Omega,\omega)\,\mathrm{e}^{-\mathrm{i}\omega t} \tag{17}$$

and

$$V(\Omega,\omega)=\frac{1}{2}\int_{-\infty}^{\infty}\mathrm{d}x\frac{x^2p(\omega)\,\mathrm{e}^{\mathrm{i}x\Omega}}{\left[\omega-\sqrt{\frac{\pi}{2}}x^2\Delta(\omega)\right]^2+\frac{\pi}{2}x^4p(\omega)^2}. \tag{18}$$

Now note that for any set of numbers c_q we have $\sum_{q,q'}c_q^*U_{q,q'}(t)c_{q'}=\frac{1}{2\pi}\int_{-\infty}^{\infty}\mathrm{d}\Omega\left|\sum_q c_q\,\mathrm{e}^{\mathrm{i}q\Omega}\right|^2W(\Omega,t)$ and so positivity of $W(\Omega,t)$ will be sufficient for positive semidefiniteness of $\hat{U}(t)$ independent of the $\hat{q}$ spectrum.

2.3. *Finding $V(\Omega,\omega)$*

The integral over x in $V(\Omega,\omega)$ can be performed explicitly. Factoring we obtain

$$V(\Omega,\omega)=\frac{1}{\pi(\Delta(\omega)^2+p(\omega)^2)}\int_{-\infty}^{\infty}\mathrm{d}x\frac{x^2p(\omega)\,\mathrm{e}^{\mathrm{i}x\Omega}}{\left|x^2-\frac{\omega}{\sqrt{\frac{\pi}{2}}(\Delta(\omega)+\mathrm{i}p(\omega))}\right|^2}. \tag{19}$$

The integral over x can be performed using the residue theorem [28] and the fact that

$$\begin{aligned}\left|x^2-\frac{\omega}{\sqrt{\frac{\pi}{2}}(\Delta(\omega)+\mathrm{i}p(\omega))}\right|^2 &= [x-\alpha(\omega)(a(\omega)+\mathrm{i}b(\omega))]\\ &[x+\alpha(\omega)(a(\omega)+\mathrm{i}b(\omega))][x-\alpha(\omega)(a(\omega)-\mathrm{i}b(\omega))]\\ &[x+\alpha(\omega)(a(\omega)-\mathrm{i}b(\omega))]\end{aligned} \tag{20}$$

where

$$\alpha(\omega)=\left[\frac{\omega^2}{2\pi(p(\omega)^2+\Delta(\omega)^2)}\right]^{1/4}, \tag{21}$$

and

$$a(\omega)=\sqrt{1+\frac{\Delta(\omega)}{\sqrt{\Delta(\omega)^2+p(\omega)^2}}},\qquad b(\omega)=\sqrt{1-\frac{\Delta(\omega)}{\sqrt{\Delta(\omega)^2+p(\omega)^2}}}.$$

Now $V(\Omega,\omega)$ is $2\pi\mathrm{i}$ times the sum of the residues of the two poles in the upper complex plane and the result is

$$V(\Omega,\omega)=\frac{1}{2}\frac{\mathrm{e}^{-|\Omega|\alpha(\omega)b(\omega)}}{\sqrt{p(\omega)^2+\Delta(\omega)^2}\alpha(\omega)}\{a(\omega)\cos[|\Omega|\alpha(\omega)a(\omega)]-b(\omega)\sin[|\Omega|\alpha(\omega)a(\omega)]\}. \tag{22}$$

2.4. *Positivity*

Now it is clear that $\hat{U}(t)$ will be positive definite if $W(\Omega,t)$ is positive for all Ω and t. This will be true in turn by Bochner's theorem [29] if $V(\Omega,\omega)$ is a positive semidefinite function in ω.

Now by definition $V(\Omega,\omega)$ is a positive semidefinite function in ω if the matrices $M_{j,k}=V(\Omega,x_j-x_k)$, $j=1,\ldots,n$ are positive semidefinite for all n and arbitrary real x_j. Defining

$$V_\epsilon(\Omega,\omega)=\frac{1}{2}\frac{\mathrm{e}^{-|\Omega|\alpha(\omega)b(\omega)}}{\sqrt{p(\omega)^2+\Delta(\omega)^2}\alpha(\omega)+\epsilon}\{a(\omega)\cos[|\Omega|\alpha(\omega)a(\omega)]-b(\omega)\sin[|\Omega|\alpha(\omega)a(\omega)]\} \tag{23}$$

and $M_{j,k}(\epsilon) = V_\epsilon(\Omega, x_j - x_k)$, it follows that $\lim_{\epsilon\to 0} V_\epsilon(\Omega,\omega) = V(\Omega,\omega)$ and $\lim_{\epsilon\to 0} M_{j,k}(\epsilon) = M_{j,k}$. In order to get $V(\Omega,\omega)$ to be positive semidefinite we will need $\alpha(\omega) \to 0$ and $p(\omega)\alpha(\omega) \to 0$ as $\omega \to 0$ in addition to $a(0) \neq 0$. We introduced the ϵ forms since under these conditions on $p(\omega)$ the matrices $M_{j,k}(\epsilon)$ unlike $M_{j,k}$ are finite on the diagonal.

Now provided that $\alpha(\omega) \to 0$ and $p(\omega)\alpha(\omega) \to 0$ as $\omega \to 0$ and $a(0) \neq 0$, the matrices $M_{j,k}(\epsilon)$ will be diagonally dominant for sufficiently small ϵ (i.e. they will obey $|M_{j,j}(\epsilon)| \geqslant \sum_{k\neq j} |M_{j,k}(\epsilon)|$). In addition, the diagonal entries of $M(\epsilon)$ are positive and these two conditions are sufficient to guarantee that $M(\epsilon)$ is positive semidefinite [30]. It follows that M is positive semidefinite. Hence, under these conditions $V(\Omega,\omega)$ is a positive semidefinite function in ω and $\hat{\rho}(t)$ will be positive semidefinite.

2.5. *Sufficient conditions*

The conditions for positive semidefiniteness of $\hat{\rho}(t)$ can be stated somewhat more clearly as

$$\lim_{\omega\to 0} \frac{\omega}{p(\omega)} = 0 \tag{24}$$

$$\lim_{\omega\to 0} \omega p(\omega) = 0 \tag{25}$$

$$\lim_{\omega\to 0} \frac{\Delta(\omega)}{\sqrt{\Delta(\omega)^2 + p(\omega)^2}} \neq -1. \tag{26}$$

The first means that if $p(\omega) \to 0$ as $\omega \to 0$ then it must do so slower than ω. The second means that if $p(\omega) \to \infty$ as $\omega \to 0$ then it must do so more slowly than ω^{-1}. The second constraint is trivial since it would be required for integrability of $p(\omega)$. The first constraint is not very limiting. The third constraint applies only to densities which are increasing with ω, and it basically requires that $\Delta(\omega)$ must approach zero faster than $p(\omega)$. Since $\Delta(\omega)$ will usually approach zero in proportion to ω this condition is mostly covered by the first condition.

The sufficient conditions derived here are much more general than any previously stated. In [11] the stated sufficient condition required $K(t) \geqslant 0$ which would mean $p(\omega)$ must be a positive semidefinite function, which is a much stronger constraint than (24). In [14] the stated sufficient conditions include $K(t)$ positive and non-increasing in addition to even stronger constraints. It should be noted however that many memory functions which fail to satisfy (24) may still yield a positive definite $\hat{\rho}(t)$. Note that (24) is much weaker than the known sufficient conditions [6] for complete positivity.

3. Eigenvalues of $\hat{U}(t)$ for density models

The Hadamard representation (8) of the propagator is clearly a useful concept since it allows one to explore dynamical effects without reference to specific initial states. However, we are not aware of any studies of this operator in the context of decoherence dynamics. Here we calculate the eigenvalues of $\hat{U}(t)$ numerically for a three state system with scaled $\hat{q}$ eigenvalues 1, 2 and 3. Equation (9) was integrated using a recently developed numerical algorithm for integrodifferential equations [27]. We consider a number of simple models for $p(\omega)$ most of which either do not satisfy the sufficient conditions or have an ill-defined $\Delta(\omega)$.

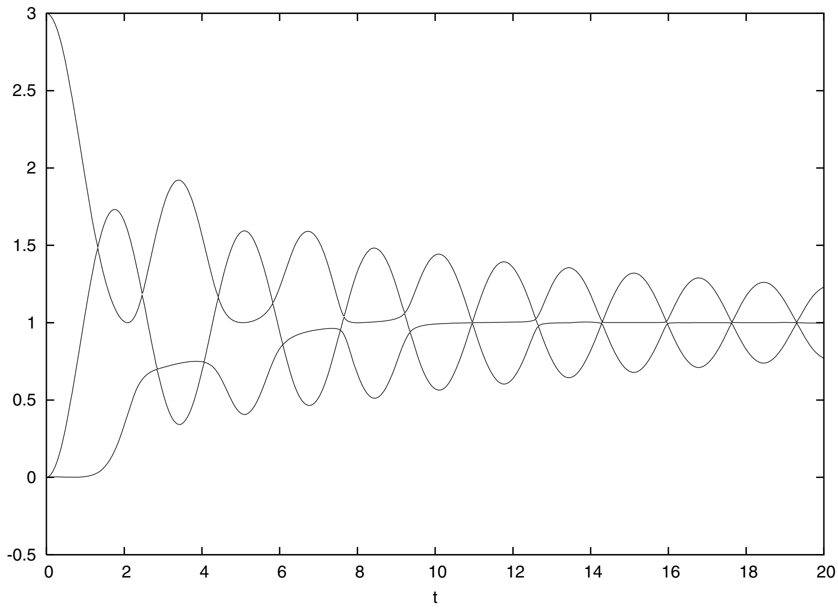

Figure 1. Eigenvalues of $\hat{U}(t)$ versus t for model 1.

3.1. Model 1: $p(\omega) = \mathrm{e}^{-\omega^2}$

This model arises from studies of complex environments [12] which treat subsystem environment interactions statistically. It satisfies the sufficient conditions and the eigenvalues of $\hat{U}(t)$ are indeed positive. The eigenvalues shown in figure 1 damp toward unity with large amplitude oscillations which means that $\hat{U}(t) \to \hat{1}$ in the limit $t \to \infty$. This means that the eigenvalues of $\hat{\rho}(t)$ in the long time limit will be the diagonal elements of $\hat{\rho}(0)$ in the $\hat{q}$ eigenbasis.

3.2. Model 2: $p(\omega) = 1/(1+\omega^2)$

This models a single resonance at the origin and corresponds to $K(t)$ of the exponential form as considered by [15]. Here again the sufficient conditions are satisfied and the eigenvalues are positive. The eigenvalues are plotted in figure 2. Decay toward unity is rapid and without significant oscillation.

3.3. Model 3: $p(\omega) = \sqrt{|\omega|}, 0 \leqslant \omega \leqslant 2$

Here the density could represent a supra ohmic bath. Here $\Delta(\omega)$ does not exist and the eigenvalues are positive. Figure 3 shows persistent oscillations in the eigenvalues which remain long after the time interval shown. (Replacement of $\sqrt{|\omega|}$ by $2\sqrt{|\omega|}$ in the model results in one negative eigenvalue.)

3.4. Model 4: $p(\omega) = |\omega|^{1/2}\,\mathrm{e}^{-\omega^2}$

Here we consider a case with non-monotonic behavior. Again $\Delta(\omega)$ does not exist and the eigenvalues are positive. Again we see decay toward unity but with an intermediate degree of damping.

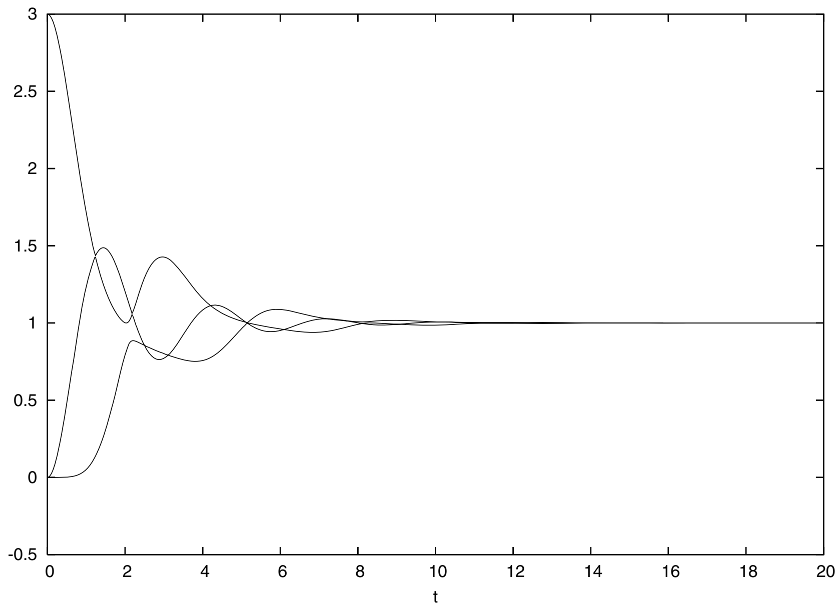

Figure 2. Eigenvalues of $\hat{U}(t)$ versus t for model 2.

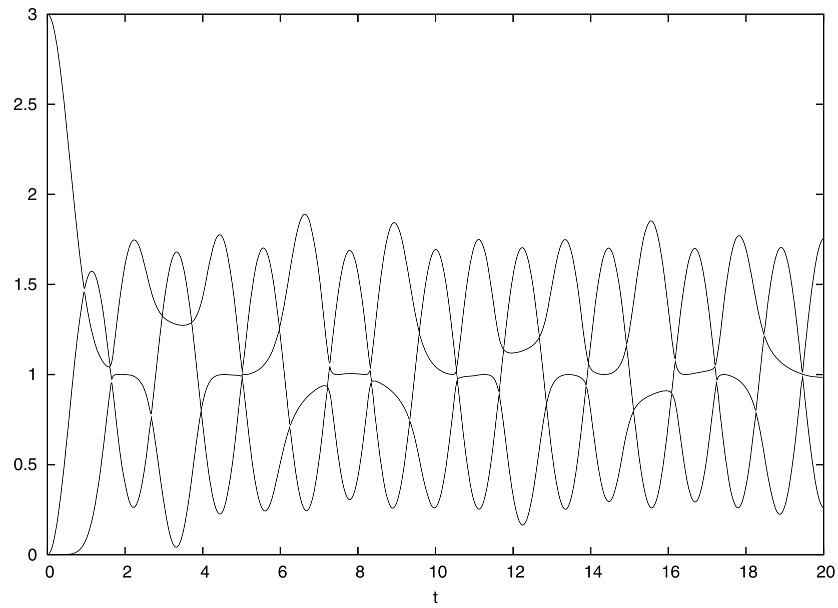

Figure 3. Eigenvalues of $\hat{U}(t)$ versus t for model 3.

3.5. Model 5: $p(\omega) = \omega^4\, e^{-\omega^2}$

This model violates conditions (24) and (26) and is also non-monotonic. Figure 5 shows that the eigenvalues are all positive and so this proves that (24) is not a necessary condition for positive

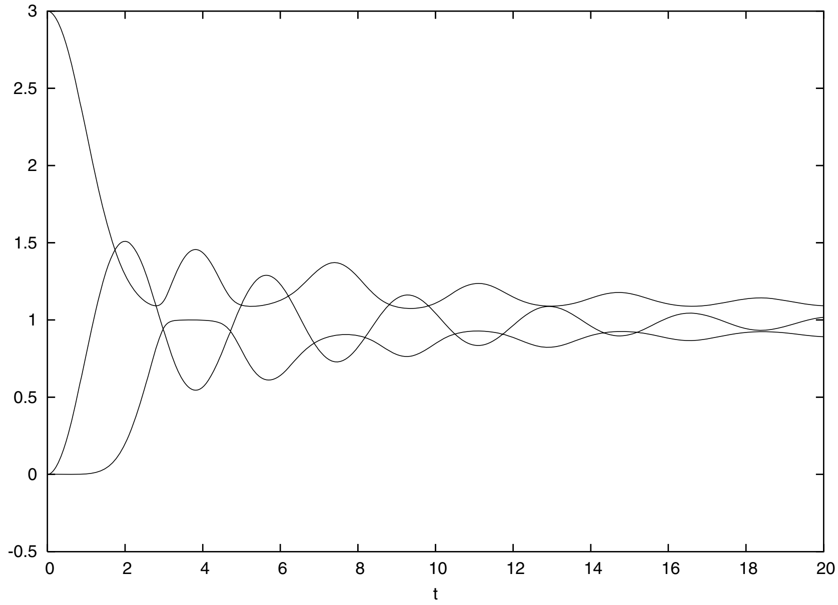

Figure 4. Eigenvalues of $\hat{U}(t)$ versus t for model 4.

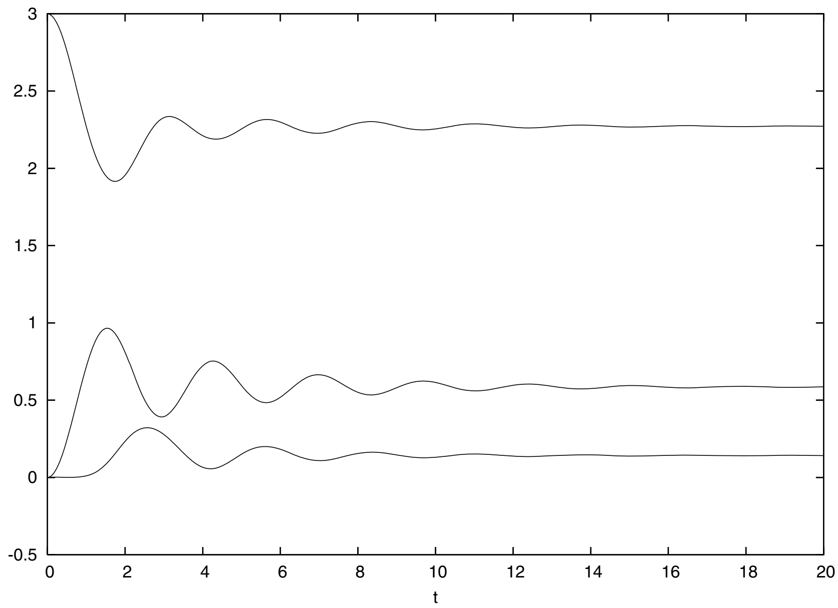

Figure 5. Eigenvalues of $\hat{U}(t)$ versus t for model 5.

semidefiniteness. An additional interesting aspect of this model is that the eigenvalues do not approach unity. This means that the eigenvalues of the density matrix in the long time limit will not be the diagonal elements of $\hat{\rho}(0)$ in the $\hat{q}$ eigenbasis. This is possible because $p(0) = 0$ for

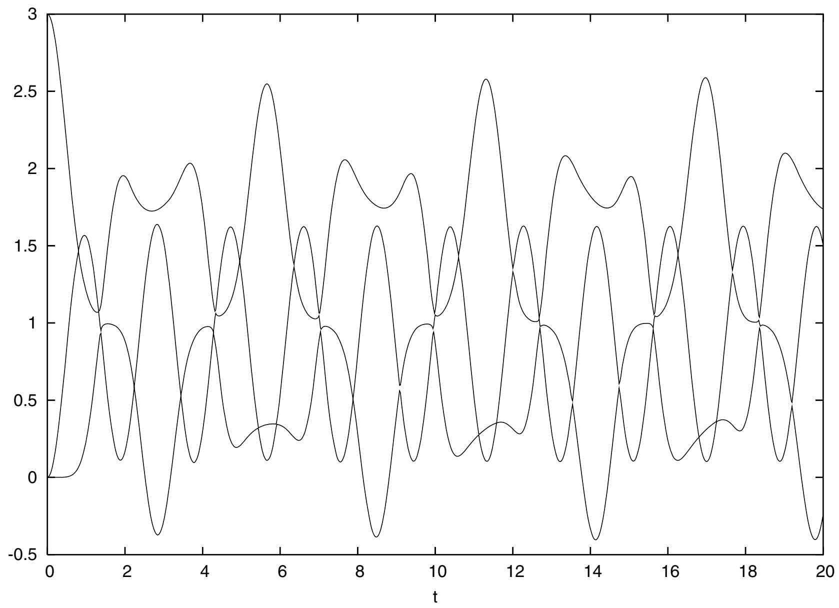

Figure 6. Eigenvalues of $\hat{U}(t)$ versus t for model 6.

this model and hence $\int_0^\infty \mathrm{d}t\, K(t) = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty}\mathrm{d}\omega \int_0^\infty \mathrm{d}t \cos\omega t = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty}\mathrm{d}\omega\, p(\omega)\pi\delta(\omega) = 0$. This then allows for the possibility of stationary off-diagonal matrix elements of $\hat{U}(t)$ in the long time limit.

3.6. Model 6: $p(\omega) = \omega^2, 0 \leqslant \omega \leqslant 2$

This Debye-type density model also violates condition (24) and it is clear from figure 6 that one of the eigenvalues is occasionally negative.

4. Summary

We have shown that non-Markovian generalizations of the Lindblad–Kossakowski master equation will preserve positivity if the generator is Hermitian and the memory function is real and can be expressed as the Fourier transform of a real positive symmetric density function $p(\omega)$ with properties (24) and (26). These sufficient conditions are more general than those previously given and they should prove to be a useful tool in the continuing efforts to generalize the Markovian Lindblad–Kossakowski [26] master equation. While the sufficient conditions were derived for evolutions without subsystem drift contributions, the analysis can be extended to this more general case using Trotter product formulae as in [14].

The analysis presented is limited to a single Hermitian generator. While it appears that Lindblad–Kossakowski operators which are sums of Hermitian generators could be treated similarly via generalized Trotter product formulae, this is not absolutely obvious and should be independently verified.

We also numerically explored the decoherence dynamics of the eigenvalues of the Hadamard propagator for a number of simple models. We were able to prove that (24) and (26) are not necessary conditions for positivity. We also found that in most cases the long time limit is the identity operator which means that the equilibrium eigenvalues of the density matrix are the diagonal elements of the initial density in the eigenbasis of the dissipative Hermitian generator. We also showed that this is not universally true. There are cases where the density $p(\omega)$ vanishes at $\omega = 0$ where the Hadamard propagator approaches a constant matrix which is not the identity. In this case the eigenvalues of the equilibrium density matrix are dynamically determined and are obviously dependent on the density $p(\omega)$. This is of particular interest because it is often assumed that non-Markovian effects are unimportant in the long time limit, while in this model they actually determine the equilibrium density.

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