Derivation of Markovian master equations for spatially correlated decoherence

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We introduce a general formalism to describe the effects of Markovian noise which is spatially correlated, typically decaying over some finite correlation length. For any system of interest, this formalism describes spatial correlations without the necessity to choose a particular microscopic model for the environment. We present a method of mapping the equations to Lindblad form and discuss functional forms for homogeneous spatial correlation functions. We also discuss two example microscopic models for the environment which exhibit nontrivial spatial-temporal correlation functions.

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I. INTRODUCTION

The study of open quantum systems and the concept of a density matrix master equation underlies much of modern quantum physics, be it quantum optics, atom optics, condensed matter physics, or quantum computation. When deriving or assuming a particular form for the master equation via the usual system-bath model [1], it is common to assume each component of a system either couples to the same bath (*correlated* or *collective* decoherence channels) or individual baths (*uncorrelated* or *independent* decoherence channels); see, e.g., [2–6]. We explore the regime between these two extremes, introducing the concept of a *correlation length* ξ and deriving a general master equation method for treating such partially correlated environments.

Decoherence induced by a correlated environment is a commonly observed effect. The concepts of super- and subradiance [7,8] and decoherence-free subspaces [9–14] rely on the interference resulting from several subsystems coupled to the same environmental mode. Even some of the foundational work on decoherence in quantum computation considered both fully correlated and uncorrelated environments [15–18]. Recently, the ramifications of correlated environments have been discussed in such diverse situations as scalable quantum error correction [2,19–24], photosynthesis and biological chromophores [25–29], and multiatom trapping experiments [30–33].

The Lindblad equation [1,34-36] is the workhorse of open quantum systems due to its simple form and well-behaved mathematical properties. Yet, deriving a general master equation of this form for (partially) correlated environments is nontrivial. Lindblad operators can be derived or assumed which act individually, pairwise, or collectively, yet how does one choose these in a physically sensible manner? We use a general Bloch-Redfield approach, where environmental noise correlation functions appear naturally in the formalism. Given sufficiently well behaved environmental correlations, a closed-form master equation can be obtained with the same form as the Lindblad equation but whose operators and rates are linked directly to the original physical system-bath Hamiltonian. Following this route we consider a generalization of the environmental correlation function which includes spatial (as well as temporal) correlations and therefore derive a general master equation. This describes spatially correlated decoherence independent of the particular bath Hamiltonian

and purely based on environmental correlation functions. We also consider two examples where such *spatial-temporal* correlation functions can be derived microscopically.

II. BLOCH-REDFIELD EQUATIONS WITH SPATIAL CORRELATIONS

We start from the usual system-bath Hamiltonian

$$H = H_S + H_B + H_{\text{int}} \tag{1}$$

comprised of system (H_S) , bath (H_B) , and the interaction between them

$$H_{\rm int} = \sum_j s_j B_j, \qquad (2)$$

where s_j are system operators and B_j bath operators. An arbitrary basis $\{|a_n\rangle\}$ and the Hamiltonian eigenstates $H_S |\omega_n\rangle = \omega_n |\omega_n\rangle$ are connected via the transformation matrix $V = \sum_n |\omega_n\rangle \langle a_n|$. A compact and general form of the Bloch-Redfield equations is then given by (see Appendix A)

$$\dot{\rho} = \frac{\iota}{\hbar} [\rho, H_s] + \frac{1}{\hbar^2} \sum_{j,k} (-s_j V q_{jk} V^{\dagger} \rho + V q_{jk} V^{\dagger} \rho s_j - \rho V \hat{q}_{jk} V^{\dagger} s_j + s_j \rho V \hat{q}_{jk} V^{\dagger})$$
(3)

with

$$\langle a_n | q_{jk} | a_m \rangle = \langle a_n | V^{\dagger} s_k V | a_m \rangle \frac{1}{2} C_{jk} (\omega_m - \omega_n), \qquad (4)$$

$$\langle a_n | \hat{q}_{jk} | a_m \rangle = \langle a_n | V^{\dagger} s_k V | a_m \rangle \frac{1}{2} C_{kj} (\omega_n - \omega_m), \qquad (5)$$

$$C_{jk}(\omega) = \int_{-\infty}^{\infty} d\tau \ e^{i\omega\tau} \langle \tilde{B}_j(\tau) \tilde{B}_k(0) \rangle.$$
 (6)

The spectral functions $C_{jk}(\omega)$ define the bath, i.e., the environment. They are given by the Fourier transform of the correlation functions of the bath operators in the interaction picture $\tilde{B}_{j}(\tau) = \exp(iH_{B}\tau)B_{j}\exp(-iH_{B}\tau)$.

A. Spatial-temporal correlations

The spectral functions define both the correlation function with increasing time difference τ and which of the pairs of bath operators B_j , B_k (corresponding to system operators s_j , s_k) are correlated. The operators B_j can be grouped such that

$$C_{jk}(\omega) = \begin{cases} C_{jk}(\omega) & \text{if } j \text{ and } k \text{ are in the same group,} \\ 0 & \text{if } j \text{ and } k \text{ are in different groups.} \end{cases}$$

This may be due to either the assumption of a certain structure in the environment or groups of different types of coupling operators (see Appendix B). We call each group an independent bath since they are not correlated with the other baths.

If the environment is thought to be a continuum with decaying correlations over increasing distances a more flexible model is to introduce a spatial dependency in the spectral function:

$$C_{jk}(\omega,\mathbf{r}_j,\mathbf{r}_k) := \int_{-\infty}^{\infty} d\tau \ e^{i\omega\tau} \langle \tilde{B}_j(\tau,\mathbf{r}_j)\tilde{B}_k(0,\mathbf{r}_k) \rangle, \quad (7)$$

where the components of the system couple to the environment at positions \mathbf{r}_j , \mathbf{r}_k . This function is similar to a Van Hove function [37]; however we use real-space coordinates rather than k space. As in conventional Bloch-Redfield theory, this spectral function can be derived from a more fundamental microscopic model or its form can be phenomenologically assumed, typically as a homogeneous spectral function $C_{jk}(\omega,\mathbf{r}_j,\mathbf{r}_k) = C(\omega,|\mathbf{r}_j - \mathbf{r}_k|)$ which will approach zero for increasing distance.

Strictly speaking the spectral function $C_{jk}(\omega)$ is actually given by a one-sided Fourier transform $D_{jk}(\omega) = C_{jk}(\omega) + iF_{jk}(\omega)$; i.e., it may be complex. Such a term would lead to additional coherent dynamics. In the secular approximation it can be written as a correction $H_S \rightarrow H_S + H_{cor}$ to the system Hamiltonian [see Eq. (C4)], where $H_{cor} = \sum_{jk} F_{jk} s_k^{\dagger} s_j$. In cases of uncorrelated decoherence (all terms for which $j \neq k$ are zero) this correction of the system Hamiltonian is generally neglected since the terms $s_j^{\dagger} s_j$ in qubit systems are diagonal in the system eigenbasis. In cases of correlated decoherence however the correction Hamiltonian H_{cor} can lead to interaction terms between the qubits, i.e., environmentally induced interactions.

B. Qubit example

As an example we apply this formalism to two uncoupled qubits $H_S = \sum_{j=1}^2 \omega_q \sigma_z^{(j)}$, each interacting longitudinally with the environment $H_{\text{int}} = \sum_{j=1}^2 \sigma_z^{(j)} B_j$. With the four states $|1,1\rangle,|1,0\rangle,|0,1\rangle,|0,0\rangle$ we find a reduced dephasing rate γ_- for the single excitation subspace $\{|1,0\rangle, |0,1\rangle\}$ and an enhanced dephasing rate γ_+ between the states $|1,1\rangle$ and $|0,0\rangle$ while all other pairs dephase at a rate γ_0 . These rates are obtained in terms of $C(\omega, |\mathbf{r}_i - \mathbf{r}_k|)$ as

$$\gamma_{-} = C(0,0) - C(0,d),$$
 (8)

$$\gamma_{+} = C(0,0) + C(0,d), \tag{9}$$

$$\gamma_0 = C(0,0)/2, \tag{10}$$

where $d = |\mathbf{r}_1 - \mathbf{r}_2|$ is the distance between the qubits. For uncorrelated decoherence only the self-correlations are nonzero and all coherences decay at the rate γ_0 or $2\gamma_0$. With increasing noise correlation length and fixed qubit distance the single excitation subspace's dephasing rate γ_- is reduced while γ_+ is increased. This reduction of γ_- is the basis of a decoherence-free subspace [9].

For *n* qubits in an uncorrelated environment the dephasing rate between two states is proportional to the number n_f of flipped qubits between the two states. In a perfectly correlated environment however the dephasing rate between two states with a difference of n_e excitations is proportional to n_e^2 and n_f is irrelevant. Therefore the dephasing rate between states with equal excitation number is reduced to zero when the noise correlation length increases well beyond the qubits' separation, forming a decoherence-free subspace. For example a coherence of the form $|0011\rangle\langle 1100|$ will decay with rate $\Gamma = n_f \gamma = 4\gamma$ for $\xi \to 0$ and as $\Gamma = n_e^2 \gamma = 0$ for $\xi \to \infty$, where γ is the corresponding single-qubit dephasing rate. In contrast, the coherence $|0000\rangle\langle 1111|$ which also decays as $\Gamma = n_f \gamma = 4\gamma$ for $\xi \to 0$ will decay as $\Gamma = n_e^2 \gamma = 16\gamma$ for $\xi \to \infty$; i.e., the rate increases immensely for long correlation length.

III. ANALYTICAL SPATIAL CORRELATION FUNCTIONS

To illustrate the concept of spatially correlated decoherence, we now consider two example microscopic models for an environment without choosing a particular system Hamiltonian. The environmental spatial-temporal correlation function as well as the spectral function can be calculated explicitly showing different spatial correlations in each example. In the first case the correlation length links naturally to the environmental parameters; in the second case the spatial correlations oscillate with increasing distance.

A. One-dimensional Ising model

The first microscopic example is one of a system dephasing due to the influence of a classical one-dimensional Ising chain of N coupled spins $S_x = \pm 1$ with Hamiltonian

$$H_B = -J \sum_{x=1}^{N-1} S_x S_{x+1}$$
(11)

with coupling strength *J*. The spatial correlations in a thermal equilibrium state are given by an exponential decay [38]

$$\langle S_x S_{x'} \rangle = \tanh^{|x-x'|}(\beta J) = \exp\{\ln[\tanh(\beta J)] |x-x'|\}$$
(12)

with $\beta = 1/k_BT$. This can be extended [39,40] to a spatialtemporal correlation function by introducing a switching rate per unit time $\alpha/2$ between the two states $S_x = \pm 1$ for each spin (due to a heat bath), leading to an infinite sum of exponential decays in space multiplied with modified Bessel function of the first kind $I_n(\tau)$ in time:

$$\langle S_x(0)S_{x'}(\tau)\rangle = \sum_{l=-\infty}^{\infty} \eta^{|x-x'+l|} I_l(\gamma \alpha |\tau|) e^{-\alpha |\tau|}, \quad (13)$$

where $\eta = \tanh(\beta J)$ and $\gamma = \tanh(\beta 2J)$. Note that setting $\tau \to 0$ in Eq. (13) yields Eq. (12).

Dephasing in qubit systems is generally caused by the noise at zero frequency and the spatial correlations at $\omega = 0$ can be calculated (assuming positive J) by integrating over each summand in Eq. (13) and evaluating the sum afterwards,

$$C(\omega = 0, |x - x'|) = \frac{2(|x - x'| + \zeta)\zeta \eta^{|x - x'|}}{\alpha}, \quad (14)$$

with $\zeta = \cosh(2J\beta)$ and $\eta = \tanh(\beta J)$. The spectral function decays with distance as $x \exp(-x)$ and with it the collective terms of the dephasing rate [cf. Eqs. (8) and (9)] decay. The effective correlation length in this example increases with the coupling J of the environmental spins and decreases with temperature k_BT . Note that the spatial indices here are natural numbers, i.e., in units of the separation between environmental Ising spins, w.

Using this spectral function for our previous example of a two-qubit system (Sec. II B) one finds the rates

$$\gamma_{-} = \frac{2\zeta}{\alpha} [\zeta - \eta^{d} (d + \zeta)], \qquad (15)$$

$$\gamma_{+} = \frac{2\zeta}{\alpha} [\zeta + \eta^{d} (d + \zeta)], \qquad (16)$$

$$\gamma_0 = \zeta^2 / \alpha, \tag{17}$$

where $\zeta = \cosh(2J\beta)$ and $\eta = \tanh(J\beta)$, and the qubit distance *d* is given in units of the environmental Ising spins' nearest-neighbor distance, *w*. For close distances $d \ll J\beta$ the correlated decoherence effects are the strongest and the reduced dephasing rate γ_{-} is close to zero.

B. Bosonic chain

One of the most studied system-bath models is the spinboson model [15,18,41–43] where a spin undergoes dephasing due to an ensemble of uncoupled harmonic oscillators. To generalize this model, we now ask the question of how two (or more) spins, located at positions x and x' (etc.), are affected by a common bath with nontrivial correlations. As an example of such a bath we consider a one-dimensional chain of spatially located, coupled harmonic oscillators, the "tight-binding chain," described by

$$H_B = \sum_{x=1}^{N} \omega_0 a_x^{\dagger} a_x - g \sum_{x=1}^{N-1} (a_x^{\dagger} a_{x+1} + a_{x+1}^{\dagger} a_x).$$
(18)

Transforming into *k* space via a lattice Fourier transform [44] diagonalizes the Hamiltonian for large *N*, $H_B = \omega_k \sum_k a_k^{\dagger} a_k$ with $\omega_k = \omega_0 - 2g \cos kw$ where *w* is the environmental lattice spacing. For a finite chain length, the sum over *k* is given by $k_n = 2\pi n/Nw$ for integer $n \in [-N/2, N/2]$.

We choose the bath operators B_j in the interaction Hamiltonian [Eq. (2)] to be the lowering and raising operators a_x, a_x^{\dagger} at a particular position x,

$$B(x) = a_x = \sum_k \frac{e^{ikxw}}{\sqrt{N}} a_k, \quad B^{\dagger}(x) = a_x^{\dagger} = \sum_k \frac{e^{-ikxw}}{\sqrt{N}} a_k^{\dagger},$$

which are nonlocal in k space [44] and similar in form to Ref. [18].

1. Spatial-temporal correlation functions

If we assume the steady-state density matrix of the harmonic oscillator chain is a fully mixed state (in the Fock basis of the k modes) we can compute the four spatial-temporal

correlation functions for a coupled chain of harmonic oscillators:

$$\langle \tilde{B}(\tau, x)\tilde{B}(0, x')\rangle = \langle \tilde{B}^{\dagger}(\tau, x)\tilde{B}^{\dagger}(0, x')\rangle = 0$$
(19)

and

$$\langle \tilde{B}^{\dagger}(\tau, x) \tilde{B}(0, x') \rangle = \sum_{k} \frac{1}{N} e^{-ik(x - x')w} e^{i\omega_{k}\tau} \langle n_{k} \rangle, \quad (20)$$

$$\langle \tilde{B}(\tau, x) \tilde{B}^{\dagger}(0, x') \rangle = \sum_{k} \frac{1}{N} e^{ik(x - x')w} e^{-i\omega_{k}\tau} (1 + \langle n_{k} \rangle), \quad (21)$$

where $\langle n_k \rangle$ is the expectation value of the occupation number of mode k. These expressions are exact and can be evaluated numerically for finite N. To obtain more physical insight we take the limits of large energies, where $\langle n_k \rangle \approx \exp(-\hbar\omega_k\beta)$, and a long chain

$$\sum_{n=-N/2}^{N/2} f(k_n) \to \frac{Nw}{2\pi} \int_{-\pi/w}^{\pi/w} dk f(k).$$
 (22)

If we assume that the correlations in the chain are dominated by propagating excitations, we may also linearize the dispersion relation $\omega_k \approx \omega_0 + 2g(|k|w - \pi/2)$ within the first Brillouin zone.

Taking these limits, we find that the correlation function decays for large τ as

$$\lim_{\tau \to \infty} \langle \tilde{B}^{\dagger}(\tau, x) \tilde{B}(0, x') \rangle \propto \frac{1}{2\pi g \tau}.$$
 (23)

This slow algebraic temporal decay indicates the potential for non-Markovian memory effects of this environment. However, the coupling strength g is an environmental parameter and in the limit where g is much larger than the relevant system parameters the decay time of correlations is much shorter than the relevant system time scales. Only in this limit the corresponding spectral function can be used for Markovian master equations.

For linearized dispersion, we can also evaluate the spatial correlations at one moment in time $t = t' \Leftrightarrow \tau = 0$, in the limit of $g\beta \gg 0$ and normalized by the value for x = x',

$$\frac{\langle \tilde{B}^{\dagger}(t,x)\tilde{B}(t,x')\rangle}{\langle \tilde{B}^{\dagger}(t,x)\tilde{B}(t,x)\rangle} = \frac{(2\beta g)^2}{(2\beta g)^2 + (x-x')^2}.$$
 (24)

This indicates that the mixed spatial correlations decay over a characteristic correlation length $\xi = 2w\beta g$, due to the interplay between excitations hopping along the chain and thermal noise.

2. Spectral functions

While the relative spatial correlation function for $\tau = 0$ shows Lorentzian decay [Eq. (24)] the spectral function shows very different spatial correlations. The spectral function of Eq. (20) can be computed in the limit of large *N*, using the identity $\delta(f(k)) = \sum_{j} \frac{\delta(k-k_j)}{|f'(k_j)|}$ where $f(k_j) = 0$. For cosine dispersion and a Boltzmann distribution for $\langle n(\omega) \rangle$ we find

$$C_{B^{\dagger}B}(\omega, x - x') = \Theta \left(2|g| - |\omega + \omega_0|\right) \\ \times \frac{\cos\left[(x - x')\arccos\left(-\frac{\omega + \omega_0}{2g}\right)\right] \langle n(|\omega|) \rangle}{\pi \sqrt{4g^2 - (\omega + \omega_0)^2}}.$$
(25)

The spectral function $C_{BB^{\dagger}}(\omega, x - x')$ corresponding to Eq. (21) takes the same form with $\omega \to -\omega$ and $\langle n(|\omega|) \rangle \to [1 + \langle n(|\omega|) \rangle]$.

The spectral functions show that the noise consists of frequencies centered around the oscillator's eigenenergies ω_0 with a noise cutoff at $\omega_0 \pm 2g$ due to the band gap of the chain. For a given frequency the spatial correlations are cosine oscillations with distance |x - x'|, allowing points of negative correlations. The cosine shape is physically necessary as the self-correlations (at |x - x| = 0) always need to be positive.

With this spectral function the rates in our previous example of a two-qubit system (Sec. II B) become

$$\gamma_{-} = [1 - \cos(d\pi/2)] / [2\pi g \langle n(0) \rangle], \qquad (26)$$

$$\gamma_{+} = [1 + \cos(d\pi/2)] / [2\pi g \langle n(0) \rangle], \qquad (27)$$

$$\gamma_0 = 1/[\pi g \langle n(0) \rangle], \tag{28}$$

where *d* is given in units of the environmental nearest-neighbor distance of the harmonic oscillators *w* and we assume $\omega_0 \approx 0$ on the scale of the system energies making their energy spectrum approximately continuous. There are now three types of system dynamics: For $\cos(d\pi/2) = 1$ one finds the qubits fully (positively) correlated and $\gamma_- \rightarrow 0$, similar to the previous model (Sec. III A) for short distances. At the points where $\cos(d\pi/2) = 0$ the collective terms are zero and all correlated decoherence effects vanish. For $\cos(d\pi/2) = -1$ the collective terms are negative and $\gamma_+ \rightarrow 0$; i.e., the reduced and enhanced rates swap roles. This means the subspace $\{|1,0\rangle, |0,1\rangle\}$ becomes decoherence free and the subspace $\{|1,0\rangle, |0,1\rangle\}$ has an enhanced dephasing rate. This rare case only occurs at points where the environmental noise of the two qubits is negatively correlated.

IV. PHENOMENOLOGICAL SPATIAL CORRELATION FUNCTIONS AND VALID FUNCTIONAL FORMS

Ideally one has a clear microscopic model of a particular environment and can derive a spatial-temporal correlation function from it. However in some cases it is necessary to assume the spatial-temporal correlations phenomenologically. We now present a method to map the Bloch-Redfield equations to Lindblad form, which provides a test of complete positivity in the time evolution for any such phenomenological spatialtemporal correlation function. We furthermore present two examples of valid functional forms.

A. Mapping to Lindblad equations

The Bloch-Redfield equations do not guarantee complete positivity by their mathematical form but depend on a consistent model of the environment's temporal and spatial correlation functions. When assuming a phenomenological spatialtemporal correlation function $C_{jk}(\omega, \mathbf{r}_j, \mathbf{r}_k)$, highly nontrivial physical conditions apply for multipartite correlations. We therefore present a way to check for a mapping to the Lindblad equations which are known to be "the most general form of the generator of a quantum dynamical semigroup" [1,34,35]. This means that the time-evolution operator due to a certain Markovian master equation is a completely positive map of the density matrix if and only if there exists a set of operators in which the master equation takes on Lindblad form.

We take the Bloch-Redfield equations in the secular approximation (see Appendix B):

$$\dot{\rho} = \frac{i}{\hbar} [\rho, H_s] + \frac{1}{\hbar^2} \sum_{j,k} C_{jk} \left(s_k \rho s_j^{\dagger} - \frac{1}{2} \{ s_j^{\dagger} s_k, \rho \} \right).$$
(29)

This equation can be mapped to Lindblad form if and only if there exists an invertible matrix W such that $W^{\dagger}C_{jk}W$ is diagonal with nonnegative eigenvalues. The eigenvalues then correspond to the Lindblad rates. The Lindblad operators are given by

$$L_k = \sum_j W_{jk} s_j. \tag{30}$$

For real-valued homogeneous correlation functions, $C_{jk}(\mathbf{r}_j, \mathbf{r}_k) = C_{jk}(|\mathbf{r}_j - \mathbf{r}_k|)$, the coefficient matrix C_{jk} is symmetric and its diagonalization is unitary; i.e., Eq. (29) can be mapped to Lindblad form if the coefficient matrix is positive semidefinite. If one or more eigenvalues are negative then according to Sylvester's law of inertia [45] all transforms $W^{\dagger}C_{jk}W$ will have the same number of negative values on the diagonal; i.e., there is no mapping to Lindblad form.

B. Valid functional forms

To illustrate this procedure, we consider a one-dimensional chain of equidistant subsystems (separated in space by a distance d). We now show that the following two functional forms can always be mapped to Lindblad form. Both are therefore sensible physical models of spatial correlations which guarantee complete positivity in the time evolution:

$$C_{jk} = \exp[-a|j-k|]$$
 exponential decay, (31)

$$C_{jk} = \exp[-a(j-k)^2]$$
 Gaussian function, (32)

where the parameter a > 0 sets the decay in terms of the environmental correlation length, $a = d/\xi$.

We first note that homogeneous coefficient matrices C_{jk} with row j and column k are Toeplitz matrices. To determine whether it is positive semidefinite we utilize Lemma 6 in Chapter 4.2 of Ref. [46], which applied to our notation reads as follows:

The eigenvalues of an $n \times n$ Hermitian Toeplitz matrix in the notation

$$(C_{jk}) = \begin{pmatrix} t_0 & t_{-1} & t_{-2} & t_{-3} & \dots & t_{-n+1} \\ t_1 & t_0 & t_{-1} & t_{-2} & \ddots & \\ t_2 & t_1 & t_0 & t_{-1} & \ddots & \\ t_3 & t_2 & t_1 & t_0 & \ddots & \\ \vdots & \ddots & \ddots & \ddots & \ddots & \vdots \\ t_{n-1} & & & \dots & t_0 \end{pmatrix}$$
(33)

with absolutely summable elements t_m ,

$$\sum_{m=-\infty}^{\infty} |t_m| < \infty, \tag{34}$$

are not smaller than the minimum and not greater than the maximum of the Fourier series $f(\lambda)$ defined by

$$f(\lambda) = \sum_{m=-\infty}^{\infty} t_m e^{-im\lambda}.$$
 (35)

1. Exponential decay

Since the element index in Eq. (33) corresponds to the difference (row – column) the Toeplitz matrix corresponding to Eq. (31) is given by the elements $u_m = e^{-a|m|}$. Via a geometric series, they are found absolutely summable:

$$\sum_{m=-\infty}^{\infty} |u_m| = 1 + 2\sum_{m=1}^{\infty} e^{-am} = \frac{2}{1 - e^{-a}} - 1 < \infty.$$
 (36)

Similarly the Fourier series evaluates to

m

$$g(\lambda) = \sum_{m=-\infty}^{\infty} u_m \exp(-im\lambda)$$
(37)

$$= -1 + \frac{2(1 - e^{-a}\cos\lambda)}{1 - 2e^{-a}\cos\lambda + e^{-2a}} > 0.$$
(38)

Since the Fourier series $g(\lambda)$ is greater than zero, the eigenvalues of the corresponding Toeplitz matrices are greater than zero. Any master equation based on an exponentially decaying spatial correlation function $C_{jk} = \exp(-a|j-k|)$ can therefore be mapped to Lindblad form.

2. Gaussian decay

The Toeplitz matrix corresponding to Eq. (32) has absolutely summable elements $v_m = e^{-am^2}$,

$$\sum_{m=-\infty}^{\infty} |v_m| = 2\sum_{m=0}^{\infty} e^{-am^2} - 1 < \infty,$$
 (39)

while the Fourier series is given by

$$h(\lambda) = \sum_{k=-\infty}^{\infty} v_k e^{ik\lambda} = 1 + 2\sum_{k=1}^{\infty} e^{-ak^2} \cos(k\lambda) > 0, \quad (40)$$

which can be shown using Jacoby's imaginary transformation (Chapter 21, page 475 of Ref. [47]). Again we see that the Fourier series $h(\lambda)$ and therefore the eigenvalues of the corresponding Toeplitz matrices are greater than zero which means that any master equation based on a Gaussian correlation function can be mapped to Lindblad form.

3. Step function

Finally we give a counterexample where the mapping fails, indicating an unphysical correlation function. The Toeplitz matrix corresponding to a step correlation function has the elements

$$w_m = \begin{cases} 1 & \text{for } |m| < 2, \\ 0 & \text{otherwise.} \end{cases}$$
(41)

The elements are absolutely summable $\sum_{m=-\infty}^{\infty} |w_m| = 3$; however the Fourier series has negative values:

$$\sum_{k=-\infty}^{\infty} w_k e^{ik\lambda} = e^{i\lambda} + e^{-i\lambda} + 1 = 1 + 2\cos\lambda.$$
 (42)

In fact for the specific case of a system consisting of three subsystems

$$\det \begin{pmatrix} 1 & 1 & 0\\ 1 & 1 & 1\\ 0 & 1 & 1 \end{pmatrix} = -1;$$
(43)

i.e., the matrix is not positive semidefinite. This 3×3 matrix is a principal submatrix [48] of the coefficient matrix for any correlation function which corresponds to a step function. Following the definiteness criterion of symmetric matrices [48,49], it follows that no step function correlation matrix (other than trivial limiting cases) is positive semidefinite. Step functions should therefore not be used as the form of a *homogeneous* spatial correlation function as they always lead to a time evolution which is not completely positive, even though the temporal component can be considered to be Markovian.

V. CONCLUSION

We have utilized the Bloch-Redfield formalism to include spatial correlations within a decohering environment. This approach is very general as the effect of the environment is modeled via spatial-temporal correlation functions.

The typical effects of spatially correlated decoherence on qubit systems are the formation of decoherence-free subspaces as well as enhanced dephasing rates between other states. For positively correlated noise the dephasing rate between two states is proportional to the square of the excitation difference of the two states.

Two microscopic examples for an environment were presented where the spatial-temporal correlation function can be derived explicitly. The one-dimensional Ising model has a purely positive spectral function which decays spatially. The spatial correlation length is increased by stronger coupling between the environmental spins and decreased by thermal effects. The chain of harmonic oscillators shows a spectral function which oscillates spatially in the form of a cosine, creating points of negative correlation.

We also provide a method for working with phenomenologically assumed spectral functions. A mapping to the completely positive Lindblad form master equation provides a test for physicality of the spectral functions in the Markovian regime. With this test we show that homogeneous exponential or Gaussian spatial decay with an arbitrary correlation length proves to be a physical model for spectral functions.

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APPENDIX A: DERIVATION OF THE MATRIX FORM OF THE BLOCH-REDFIELD EQUATIONS

The derivation of the Bloch-Redfield equations [50-52] is a well known procedure which can be found in several good textbooks [1,36,53]. In this and the following appendices, we summarize this derivation and its associated results for two reasons, first to clarify our notation and form of the equations and second to discuss several important approximations explicitly. Although these approximations are included in the usual discussions, the introduction of spatial correlations requires careful treatment of these points.

From the usual system-plus-bath approach,

$$H = H_S + H_B + H_{\text{int}}$$
 with $H_{\text{int}} = \sum_j s_j B_j$,

where the interaction is given as a product of system operators s_j and bath operators B_j , one finds the standard master equation in the Born-Markov approximation [see, e.g., Carmichael [36], Eq. (1.34)]:

$$\begin{split} \dot{\hat{\rho}} &= \sum_{jk} \int_0^\infty dt' [\tilde{s}_j(t)\tilde{s}_k(t')\tilde{\rho} - \tilde{s}_k(t')\tilde{\rho}\tilde{s}_j(t)] \langle \tilde{B}_j(t)\tilde{B}_k(t') \rangle \\ &+ \sum_{jk} \int_0^\infty dt' [\tilde{\rho}\tilde{s}_k(t')\tilde{s}_j(t) - \tilde{s}_j(t)\tilde{\rho}\tilde{s}_k(t')] \langle \tilde{B}_k(t')\tilde{B}_j(t) \rangle, \end{split}$$

where the tilde implies the interaction picture. To define our matrix notation in an arbitrary basis $\{|a_n\rangle\}$ we introduce the transformation matrix $V = \sum_n |\omega_n\rangle \langle a_n|$ to the system Hamiltonian's eigenstates $H_S |\omega_n\rangle = \omega_n |\omega_n\rangle$. To perform the t' integration explicitly, we transform back to the Schrödinger picture. For the first term it reads explicitly

$$s_j V \underbrace{V^{\dagger} e^{-iH_S \tau} s_k e^{iH_S \tau} V}_{=:O} V^{\dagger} \rho(t)$$
(A1)

with $\tau = t - t'$. Inserting unity operators $\sum_{n} |\omega_n\rangle \langle \omega_n|$ gives

$$Q = \sum_{lmnp} |a_l\rangle \underbrace{\langle \omega_l | e^{-iH_S\tau} | \omega_m \rangle}_{=e^{-i\omega_l\tau}\delta_{lm}} \langle \omega_m | s_k | \omega_n \rangle$$
$$\times \underbrace{\langle \omega_n | e^{iH_S\tau} | \omega_p \rangle}_{=e^{i\omega_n\tau}\delta_{np}} \langle a_p | \tag{A2}$$

$$= \sum_{mn} |a_m\rangle \langle \omega_m| s_k |\omega_n\rangle \langle a_n| e^{i(\omega_n - \omega_m)\tau}, \quad (A3)$$

$$\langle a_m | Q | a_n \rangle = \langle \omega_m | s_k | \omega_n \rangle e^{i(\omega_n - \omega_m)\tau}$$
(A4)

$$= \langle a_m | V^{\dagger} s_k V | a_n \rangle e^{i(\omega_n - \omega_m)\tau}.$$
 (A5)

Performing these operations analogously on all four terms we can then integrate element-wise and we find a compact and general form of the Bloch-Redfield equations:

$$\dot{\rho} = \frac{i}{\hbar} [\rho, H_s] + \frac{1}{\hbar^2} \sum_{j,k} (-s_j V q_{jk} V^{\dagger} \rho + V q_{jk} V^{\dagger} \rho s_j - \rho V \hat{q}_{jk} V^{\dagger} s_j + s_j \rho V \hat{q}_{jk} V^{\dagger})$$
(A6)

with

$$\langle a_n | q_{jk} | a_m \rangle = \langle a_n | V^{\dagger} s_k V | a_m \rangle D_{jk}(\omega_m - \omega_n),$$
 (A7)

$$\langle a_n | \hat{q}_{jk} | a_m \rangle = \langle a_n | V^{\dagger} s_k V | a_m \rangle D^*_{jk} (\omega_n - \omega_m), \qquad (A8)$$

$$D_{jk}(\omega) = \int_0^\infty d\tau \ e^{i\omega\tau} \ \langle \tilde{B}_j(\tau) \tilde{B}_k(0) \rangle. \tag{A9}$$

If $D_{jk}(\omega)$ contains an imaginary term, this leads to additional coherent dynamics (which in the secular approximation can

even be written as a correction of the system Hamiltonian (see section "Complex spectral functions"); therefore only the real part of D_{jk} causes decoherence. Assuming the property $\langle \tilde{B}_j(-\tau)\tilde{B}_k(0)\rangle = [\langle \tilde{B}_j(\tau)\tilde{B}_k(0)\rangle]^*$ this real part can be rewritten in terms of the Fourier transform:

$$\operatorname{Re}(D_{jk}) = \frac{1}{2}C_{jk},\tag{A10}$$

$$C_{jk}(\omega) = \int_{-\infty}^{\infty} d\tau \ e^{i\omega\tau} \langle \tilde{B}_j(\tau)\tilde{B}_k(0)\rangle.$$
(A11)

The Markov approximation, which is used to derive the Bloch-Redfield equations, requires $C_{jk}(\omega)$ to be constant on the frequency scale of the quantum system, i.e. "smoothness." This means a fast decay of the *temporal* correlation function, which is independent of the *spatial* correlation length.

APPENDIX B: SECULAR APPROXIMATION OF THE BLOCH-REDFIELD EQUATIONS

The secular approximation can be used to simplify the Bloch-Redfield equations to the form of Eq. (29). First we separate the system operators s_j into several operators by multiplication with projection operators onto the Hamiltonian eigenstates $|\omega_n\rangle$:

$$s_{j}(\epsilon) = \sum_{\omega_{m} - \omega_{n} = \epsilon} |\omega_{n}\rangle \langle \omega_{n}| s_{j} |\omega_{m}\rangle \langle \omega_{m}|.$$
(B1)

The sum extends over all Hamiltonian eigenvalues ω_n and ω_m with a fixed difference ϵ . Assuming all s_j to be Hermitian we find

$$s_j(-\epsilon) = s_j(\epsilon)^{\dagger}.$$
 (B2)

Using Eq. (B1), we write

$$s_j = \sum_{\epsilon} s_j(\epsilon),$$
 (B3)

$$q_{jk} = V^{\dagger} \sum_{\epsilon} s_k(\epsilon) \frac{1}{2} C_{jk}(\epsilon) V, \qquad (B4)$$

$$\hat{q}_{jk} = V^{\dagger} \sum_{\epsilon} s_k(\epsilon) \frac{1}{2} C_{kj}(-\epsilon) V.$$
 (B5)

Replacing Eqs. (B3) to (B5) in the Bloch-Redfield equations [Eq. (3)] and changing to the interaction picture,

$$e^{iH_{S}t}s_{j}(\epsilon)e^{-iH_{S}t} = e^{-i\epsilon t}s_{j}(\epsilon), \tag{B6}$$

one then finds

Å

$$\begin{split} \dot{\tilde{\rho}} &= \sum_{jk\epsilon\epsilon'} e^{-i(\epsilon+\epsilon')t} C_{jk}(\epsilon) [-s_j(\epsilon')s_k(\epsilon)\tilde{\rho} + s_k(\epsilon)\tilde{\rho}s_j(\epsilon')] \\ &+ \sum_{jk\epsilon\epsilon'} e^{-i(\epsilon+\epsilon')t} C_{kj}(-\epsilon) [-\tilde{\rho}s_k(\epsilon)s_j(\epsilon') + s_j(\epsilon')\tilde{\rho}s_k(\epsilon)]. \end{split}$$

Since ϵ includes negative frequencies the only nonoscillating terms are for $\epsilon' = -\epsilon$. In the secular approximation, the oscillating terms which are neglected are fast oscillating on the time scale of the system dynamics. This time scale $\tau_S = 1/|\epsilon - \epsilon'|$ for $\epsilon \neq \epsilon'$ must be much shorter than the decoherence time scale set by the terms C_{jk} and the magnitudes of the s_j . Roughly this can be restated as $H_S \gg H_{\text{int}}$. Applying

the secular approximation one finds

$$\dot{\tilde{\rho}} = \sum_{jk\epsilon} C_{jk}(\epsilon) [-s_j(-\epsilon)s_k(\epsilon)\tilde{\rho} + s_k(\epsilon)\tilde{\rho}s_j(-\epsilon)] + \sum_{jk\epsilon} C_{kj}(-\epsilon) [-\tilde{\rho}s_k(\epsilon)s_j(-\epsilon) + s_j(-\epsilon)\tilde{\rho}s_k(\epsilon)].$$
(B7)

Since the sum over ϵ extends over all positive and negative energy differences we can replace $\epsilon \rightarrow -\epsilon$ in the second line of Eq. (B7). Note that this makes the last two terms the Hermitian conjugate of the first two terms. Furthermore we swap the equivalent indices j and k in the last two terms. This together with Eq. (B2) yields

$$\dot{\tilde{\rho}} = \sum_{\epsilon} \sum_{jk} \frac{1}{2} C_{jk}(\epsilon) [2s_k(\epsilon)\tilde{\rho}s_j(\epsilon)^{\dagger} - \{s_j(\epsilon)^{\dagger}s_k(\epsilon), \tilde{\rho}\}].$$
(B8)

In several cases one finds only one frequency in the elements of q_{jk} and \hat{q}_{jk} in which case the summation over ϵ contains only one summand and can be omitted, simplifying Eq. (B8) (back in the Schrödinger picture) to

$$\dot{\rho} = \frac{i}{\hbar} [\rho, H_s] + \frac{1}{\hbar^2} \sum_{j,k} \frac{1}{2} C_{jk} (2s_k \rho s_j^{\dagger} - \{s_j^{\dagger} s_k, \rho\}).$$
(B9)

For ease of notation, the form of Eq. (B9) is used without loss of generality. For cases where the summation over ϵ in Eq. (B8) is relevant, each frequency component is added independently and all further results apply analogously. In practice the secular approximation for a particular system is best applied via the method given in Appendix A1 of Ref. [6]. The general arguments above are analogous to the derivation of the Lindblad form on pages 128ff. in Ref. [1].

For a system of two qubits

$$H = \omega_q \sigma_z^{(q1)} + (\omega_q + \delta) \sigma_z^{(q2)} + H_c,$$

the general coupling operator H_c between the two (which consists of tensor products of all Pauli matrices acting on one qubit with all Pauli matrices on the other with respective coupling strengths) can be simplified via a rotating wave approximation (assuming ω_q much greater than δ and all coupling strengths) to only a transverse and a longitudinal component:

$$H_{c} = v_{\perp} \left(\sigma_{x}^{(q1)} \sigma_{x}^{(q2)} + \sigma_{y}^{(q1)} \sigma_{y}^{(q2)} \right) / 2 + v_{\parallel} \sigma_{z}^{(q1)} \sigma_{z}^{(q2)}$$

= $v_{\perp} (\sigma_{+}^{(q1)} \sigma_{-}^{(q2)} + \sigma_{-}^{(q1)} \sigma_{+}^{(q2)}) + v_{\parallel} \sigma_{z}^{(q1)} \sigma_{z}^{(q2)}.$ (B10)

Regarding environmental coupling of a qubit the transverse component leads to energy exchange between qubit and environment and the longitudinal component simply imparts a phase shift on the qubit. The environmental coupling of the two qubits with transverse and longitudinal components is

$$H_{int} = \sigma_x^{(q1)} B_1 + \sigma_z^{(q2)} B_2 + \sigma_x^{(q2)} B_3 + \sigma_z^{(q2)} B_4.$$

Applying the secular approximation (based on a large ω_q) one finds that the two coupling types can be approximated as coupling to independent baths. For systems of several qubits this applies independently for each pair. Therefore no mixed couplings of transversal and longitudinal operators appear in the Bloch-Redfield equations in the secular approximation.

APPENDIX C: COMPLEX SPECTRAL FUNCTIONS

Strictly speaking the spectral function $C_{jk}(\omega)$ is actually given by a one-sided Fourier transform [see Eq. (A9)] $D_{jk}(\omega) = C_{jk}(\omega) + iF_{jk}(\omega)$ which can be in general complex. Taking that into account Eq. (B7) becomes

$$\dot{\tilde{\rho}} = \sum_{jk\epsilon} D_{jk}(\epsilon) [-s_j(-\epsilon)s_k(\epsilon)\tilde{\rho} + s_k(\epsilon)\tilde{\rho}s_j(-\epsilon)]$$
(C1)
+
$$\sum_{jk\epsilon} [D_{jk}(\epsilon)]^* [-\tilde{\rho}s_j(-\epsilon)s_k(\epsilon)\tilde{\rho}s_j(-\epsilon)]$$
(C2)

$$+\sum_{jk\epsilon} [D_{jk}(\epsilon)]^* [-\tilde{\rho}s_k(-\epsilon)s_j(\epsilon) + s_j(\epsilon)\tilde{\rho}s_k(-\epsilon)].$$
(C2)

Dividing the expression into its real and imaginary components, one finds additional terms to Eq. (B8):

$$\dot{\tilde{\rho}} = \sum_{\epsilon} \sum_{jk} \frac{1}{2} C_{jk}(\epsilon) [2s_k(\epsilon) \tilde{\rho} s_j(\epsilon)^{\dagger} - \{s_j(\epsilon)^{\dagger} s_k(\epsilon), \tilde{\rho}\}] + \sum_{\epsilon} \sum_{jk} i F_{jk}(\epsilon) [\rho s_j(\epsilon)^{\dagger} s_k(\epsilon) - s_j(\epsilon)^{\dagger} s_k(\epsilon) \rho], \quad (C3)$$

which (back in the Schrödinger picture) can be regarded as a correction to the system Hamiltonian, often referred to as Lamb shift terms [1]:

$$\dot{\rho} = \frac{i}{\hbar} [\rho, H_s + H_{cor}] + \frac{1}{\hbar^2} \sum_{\epsilon} \sum_{jk} \frac{1}{2} C_{jk}(\epsilon) [2s_k(\epsilon)\tilde{\rho}s_j(\epsilon)^{\dagger} - \{s_j(\epsilon)^{\dagger}s_k(\epsilon), \tilde{\rho}\}],$$
(C4)

$$H_{\rm cor} = \frac{1}{\hbar} \sum_{\epsilon} \sum_{jk} F_{jk}(\epsilon) s_j(\epsilon)^{\dagger} s_k(\epsilon).$$
(C5)

Again for ease of notation the summation over ϵ is omitted in the main text.

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