Filter Functions for Quantum Processes under Correlated Noise

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Many qubit implementations are afflicted by correlated noise not captured by standard theoretical tools that are based on Markov approximations. While independent gate operations are a key concept for quantum computing, it is actually not possible to fully describe noisy gates locally in time if noise is correlated on times longer than their duration. To address this issue, we develop a method based on the filter function formalism to perturbatively compute quantum processes in the presence of correlated classical noise. We derive a composition rule for the filter function of a sequence of gates in terms of those of the individual gates. The joint filter function allows us to efficiently compute the quantum process of the whole sequence. Moreover, we show that correlation terms arise which capture the effects of the concatenation and, thus, yield insight into the effect of noise correlations on gate sequences. Our generalization of the filter function formalism enables both qualitative and quantitative studies of algorithms and state-of-the-art tools widely used for the experimental verification of gate fidelities like randomized benchmarking, even in the presence of noise correlations.

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Introduction.—A key concept in gate-based quantum computing is the composition of algorithms from a universal set of quantum gates. In real physical devices, gate implementations are subject to noise that causes decoherence and gate errors. If this noise is uncorrelated on timescales larger than the gate duration, each gate can still be described individually by a quantum operation acting on density matrices. A closely related approach is the use of a master equation in Lindblad form [1], which governs the dynamics of density matrices under the influence of Markovian noise (defined, here, as noise that is uncorrelated on the time scale of the system dynamics).

However, the assumption of uncorrelated noise is often unjustified. A prominent example is 1/f noise characteristic for flux noise in superconducting qubits and electrical noise in quantum dot qubits and ion trap qubits, which are among the most important types of noise for solid state qubits [2–5]. Hence, the standard tools for mathematically describing gate operations are not suited for capturing experimentally relevant effects that are important for understanding the capabilities of quantum computing systems. Furthermore, the process description of a gate sequence can deviate from the concatenation of the individual gates' processes. For example, one may expect the fidelity requirements for quantum error correction to be more stringent for correlated noise as errors of different gates can interfere constructively [6].

Here, we present an intuitive and computationally efficient method based on the filter function (FF) formalism 10–7]] that overcomes these limitations for the purpose of computing process descriptions for arbitrary sequences of

gate operations subject to correlated, classical Gaussian noise. This makes our approach attractive for studying the noise properties of quantum algorithms as we demonstrate with a simple example. Because widely used tools for the experimental verification of gate fidelities, such as gate set tomography and randomized benchmarking, rely on gate sequences, our approach can also shed light on the applicability of these protocols in the presence of correlated classical noise [11–13] which violates a core assumption of standard derivations [14,15]. Furthermore, our approach captures corresponding corrections in terms of FFs.

FFs were originally introduced to compute the decay of phase coherence under dynamical decoupling sequences [16–19] consisting of wait times and perfect π pulses. For small noise strengths, they were perturbatively extended to quantum gates [20–23] to compute gate fidelities [21,22,24] and develop strategies for noise mitigation [11,25–27]. Here, we build on these results to compute quantum processes for gates and gate sequences on an arbitrary number of qubits and to analyze their concatenation properties. Relevant quantities like fidelities, measurement statistics, and leakage can be extracted from process descriptions or directly from corresponding filter functions. For ease of adoption, we also provide an easy-to-use PYTHON software package [28,29].

Quantum processes.—We begin by deriving an approximate form of the average quantum process of a quantum gate of duration τ in the presence of arbitrary classical noise. Our approach builds on the fidelity calculations of [20,21], which we briefly review and generalize in some points. Concretely, we consider a system described by the

Hamiltonian $H(t) = H_c(t) + H_n(t)$. The arbitrary, time-dependent control Hamiltonian $H_c(t)$ generates the desired unitary evolution $U_c(t)$. This evolution is perturbed by the noise Hamiltonian $H_n(t) = \sum_{\alpha} b_{\alpha}(t) B_{\alpha}(t)$ which contains zero-mean, independent and identically distributed, classical Gaussian noise variables $b_{\alpha}(t)$. We generalize beyond earlier work by additionally allowing for a deterministic time dependence of the noise operators $B_{\alpha}(t)$ in \tilde{H}_n but, for simplicity, restrict ourselves to independent noise sources α and refer to Ref. [28] for the straightforward extension to cross-correlated noise.

Next, we write the propagator for H(t) as $U(t) = U_c(t)\tilde{U}(t)$ where the unitary error propagator $\tilde{U}(t)$ contains the effect of a specific noise realization. We transform H_n to the interaction picture with respect to the control Hamiltonian, $\tilde{H}_n(t) \coloneqq U_c^\dagger(t) H_n(t) U_c(t)$, so that $\tilde{U}(t)$ satisfies i $\mathrm{d}\tilde{U}(t)/\mathrm{d}t = \tilde{H}_n(t)\tilde{U}(t)$. Note that we set $\hbar=1$ and denote operators in the interaction picture by a tilde throughout this Letter. $\tilde{U}(t=\tau) \equiv \tilde{U}$ can be generated by an effective Hamiltonian H_{eff} without explicit time dependence, $\tilde{U} = \exp(-\mathrm{i}H_{\mathrm{eff}}\tau)$.

This effective Hamiltonian can be expanded using the Magnus expansion (ME) $H_{\rm eff} = \sum_{\mu=1}^{\infty} H_{\rm eff,\mu}$. Since the ME preserves the algebraic structure of the expanded quantity, $H_{\rm eff}$ remains Hermitian even after truncating the series, allowing us to neglect contributions from higher orders. The first and second ME term are given by $H_{\rm eff,1} = 1/\tau \int_0^\tau {\rm d}t \tilde{H}_n(t)$ and $H_{\rm eff,2} = -{\rm i}/2\tau \int_0^\tau {\rm d}t_1 \int_0^{t_1} {\rm d}t_2 [\tilde{H}_n(t_1), \tilde{H}_n(t_2)]$, respectively [30,31]. Higher orders provide diminishing contributions if the noise strength $\xi := \sum_{\alpha} \|B_{\alpha}\| \sigma_{\alpha} \tau \ll 1$, where $\sigma_{\alpha} = \langle b_{\alpha}(0)^2 \rangle^{1/2}$ is the standard deviation of the noise, because they include an increasing number of factors of \tilde{H}_n which we assumed to be small [32]. This may be interpreted as the condition that the angle by which a specific noise realization $b_{\alpha}(t)$ has rotated the (generalized) Bloch vector away from its intended trajectory after time τ must be small.

We proceed beyond the works by Green *et al.* [20], where \tilde{U} was used to compute the gate fidelity, to compute the full, noise-averaged quantum process $\tilde{U}(\rho) \coloneqq \langle \tilde{U} \rho \tilde{U}^{\dagger} \rangle$. We expand the error propagator \tilde{U} in a Taylor series, keeping terms up to and including $\mathcal{O}(\xi^2)$, which yields (see, also, Refs. [33,34]),

$$\begin{split} \frac{\tilde{\mathcal{U}}(\rho) - \rho}{\tau} &= -\mathrm{i}\langle [H_{\mathrm{eff},2}, \rho] \rangle \\ &+ \tau \langle H_{\mathrm{eff},1} \rho H_{\mathrm{eff},1} - \frac{1}{2} \{H_{\mathrm{eff},1}^2, \rho\} \rangle + \mathcal{O}(\xi^4), \ (1) \end{split}$$

where square (curly) brackets denote the (anti-) commutator and $\langle \bullet \rangle$ represents averaging over noise realizations. We have already dropped terms that vanish after performing the average either due to $\langle H_{\rm eff,1} \rangle = 0$ or because correlation functions evaluated at an odd number of time

points vanish for zero-mean Gaussian noise. The form of Eq. (1) is reminiscent of a master equation in Lindblad form with Hamiltonian $H_{\rm eff,2}$ and jump operators $H_{\rm eff,1}$ with associated decay rate τ . However, instead of a differential equation governing the time evolution of ρ , it represents a finite difference equation with ${\rm d}\rho/{\rm d}t \to \Delta\rho/\tau$ that describes the average evolution after the time τ at which the gate has completed. For a single qubit, $H_{\rm eff,2}$ generates a rotation, whereas the terms involving $H_{\rm eff,1}$ correspond to a deformation of the Bloch sphere into an ellipsoid.

While it is possible to evaluate both first and second order ME terms, it is more computationally involved to calculate the nested integrals contained in $H_{\rm eff,2}$ (see Ref. [21] for an explicit treatment of higher orders). However, we argue that these terms are of less interest in typical use cases. First, they vanish under the trace and, hence, do not contribute to the fidelity of the quantum operation, $\mathcal{F} \propto \text{tr} \tilde{\mathcal{U}}$. Furthermore, second order ME terms represent the unitary (Hamiltonian) part of Eq. (1) that can be canceled to leading order by a unitary rotation as commutators of $H_{\mathrm{eff,1}}$ and $H_{\mathrm{eff,2}}$ are $\mathcal{O}(\xi^3)$. Thus, it is possible to calculate $\tilde{\mathcal{U}}(\rho)$ up to a unitary rotation just by using first order ME terms. In many contexts, this is sufficient since unitary errors are typically calibrated out in experiments, using a variety of methods [15,35–39]. However, our work shows that, even if all individual gates are perfectly calibrated, a sequence of gates might incur an additional unitary error not removed by individual calibration. Moreover, calibration procedures using gate sequences may be affected by noise-induced coherent errors. To study such effects, second order ME terms can be evaluated following a procedure we lay out in Ref. [28]. Finally, we note that truncating the expansion in Eq. (1) can, in principle, lead to unphysical dynamics, in the sense that the truncated map is not completely positive (CP) [40]. In practice, this should not pose a relevant limitation because $\tilde{\mathcal{U}}(\rho)$ differs from the true final state by terms of $\mathcal{O}(\xi^4)$, leading to errors of the same order in measurement results. Thus, unphysical errors should be small as long as the perturbative expansion is well defined. We have verified this hypothesis in (random) numerical experiments and found negative Choi eigenvalues [41] to be comparatively small in magnitude, should they occur at all.

For Gaussian noise, it is possible to go beyond our perturbative treatment via an exact solution requiring only first and second order ME terms by applying the method of cumulant expansions to a stochastic Liouville equation [28]. As it turns out, this solution is simply the matrix exponential of the superoperator form of Eq. (1), so that the latter takes on the role of the generator. Because Eq. (1) is in Lindblad form, it follows that its exponential is a CP map [42]. Thus, while the exact solution guarantees a physical output state, one loses qualitative insight into contributions from, for instance, different noise operators B_{α} because the matrix exponential can, in general, only be evaluated

numerically. Further details, including the evaluation of second order ME terms, are given in our related work [28]. Here, we focus on the nonunitary part of the weak-noise approximation Eq. (1) and, now, describe how to evaluate it.

We turn to the FF formalism and express correlation functions of noise variables by their power spectral density and the evolution of the interaction picture noise operators by their FFs in the Fourier domain. Expanding $\tilde{H}_n(t) = \sum_{\alpha} b_{\alpha}(t) \tilde{B}_{\alpha}(t)$ in a Hermitian and orthonormal operator basis $\{\sigma_k\}_{k=0}^{d^2-1}$ satisfying $\sigma_k^{\dagger} = \sigma_k$ and $\operatorname{tr}(\sigma_k \sigma_l) = \delta_{kl}$, we obtain

$$\tilde{H}_n(t) = \sum_{\alpha k} b_{\alpha}(t) \tilde{\mathcal{B}}_{\alpha k}(t) \sigma_k. \tag{2}$$

A simple choice for the σ_k is the *n*-qubit Pauli basis $\{1, \sigma_x, \sigma_y, \sigma_z\}^{\otimes n}$ which we use in the following. We identify the coefficients of the expansion,

$$\tilde{\mathcal{B}}_{\alpha k}(t) = \text{tr}[\tilde{B}_{\alpha}(t)\sigma_{k}] = \text{tr}[U_{c}^{\dagger}(t)B_{\alpha}(t)U_{c}(t)\sigma_{k}], \quad (3)$$

as the control matrix from Ref. [21] (which is related to the Pauli transfer matrix representation of a quantum process). Inserting Eq. (2) into the effective master equation Eq. (1) and dropping second order ME terms as justified above, we find

$$\tilde{\mathcal{U}}(\rho) - \rho \approx \sum_{\alpha} \sum_{kl} \Gamma_{\alpha,kl} \left(\sigma_k \rho \sigma_l - \frac{1}{2} \{ \sigma_k \sigma_l, \rho \} \right), \quad (4)$$

with the matrix of decay amplitudes Γ_{α} with entries

$$\Gamma_{\alpha,kl} = \int_0^{\tau} \int_0^{\tau} dt_1 dt_2 \langle b_{\alpha}(t_1) b_{\alpha}(t_2) \rangle \tilde{\mathcal{B}}_{\alpha k}(t_1) \tilde{\mathcal{B}}_{\alpha l}(t_2).$$
 (5)

With this basis expansion, we have transformed the effective master equation to a basis in which the jump operators σ_k are time independent, and only the decay amplitudes are functions of the internal dynamics of the gate and the noise. Hence, we can carry out the integration not on the operator level of the effective master equation, but on the level of the decay amplitudes Γ_α . This allows us to employ the FF formalism to evaluate Γ_α in Fourier space. We define the two-sided noise spectral density $S_\alpha(\omega)$ as the Fourier transform of the autocorrelation function of the noise variable $b_\alpha(t)$ via

$$\langle b_{\alpha}(t_1)b_{\alpha}(t_2)\rangle = \int_{-\infty}^{\infty} \frac{\mathrm{d}\omega}{2\pi} S_{\alpha}(\omega) \mathrm{e}^{-\mathrm{i}\omega(t_1-t_2)},$$
 (6)

where we assume that the noise is wide-sense stationary. Inserting into Eq. (5) yields

$$\Gamma_{\alpha,kl} = \int_{-\infty}^{\infty} \frac{\mathrm{d}\omega}{2\pi} S_{\alpha}(\omega) \tilde{\mathcal{B}}_{\alpha k}^{*}(\omega) \tilde{\mathcal{B}}_{\alpha l}(\omega), \tag{7}$$

with $\tilde{\mathcal{B}}_{\alpha k}(\omega) = \int_0^\tau \mathrm{d}t \tilde{\mathcal{B}}_{\alpha k}(t) e^{\mathrm{i}\omega t}$. The generalized FF $F_{\alpha,kl}(\omega) = \tilde{\mathcal{B}}_{\alpha k}^*(\omega) \tilde{\mathcal{B}}_{\alpha l}(\omega)$ describes the sensitivity of the decay amplitudes $\Gamma_{\alpha,kl}$ to noise source α at frequency ω . Now, we can use Eq. (4) together with Eq. (7) to obtain the quantum process $\tilde{\mathcal{U}}(\rho)$ generated by all noise sources up to first order ME and second order in ξ .

Given $\tilde{\mathcal{U}}$, it is straightforward to calculate key figures of merit for quantum gate operations like gate fidelity, leakage (i.e., the probability to leave the subspace of valid computational states of a physical system whose Hilbert space is often larger than the computational subspace), the diamond distance to the identity, or expectation values of measurements based on known relations, as we lay out in detail in Refs. [28,43]. It is also possible to define specific FFs that allow us to directly compute these quantities from the spectral density. For example, consider the average gate fidelity to the identity [49,50] given by $\mathcal{F} = (\operatorname{tr} \tilde{\mathcal{U}} + d)/d(d+1)$ for whose evaluation only first order Magnus terms are relevant [cf. Eq. (1)]. We obtain

$$\mathcal{F} = 1 - \frac{1}{d+1} \sum_{\alpha k} \Gamma_{\alpha,kk},\tag{8}$$

where, in line with previous literature [20,21], we can identify the fidelity FF up to first order ME as $F_{\alpha}(\omega) = \sum_{k} |\tilde{\mathcal{B}}_{\alpha k}(\omega)|^2$ which captures the fidelity's susceptibility to noise source α at frequency ω .

Filter functions of gate sequences.—Now, we show that the interaction picture noise operators \tilde{B}_{α} for concatenated gates follow a simple composition rule that arises because subsequent gates update the frame of reference for the interaction picture. In the frequency domain, the total noise operators can be described as linear combinations of the single-gate noise operators, each multiplied with a phase factor corresponding to the gates' temporal positions. Since filter functions are quadratic in the noise operators, there arise correlation terms between FFs at different positions in a gate sequence which constitute corrections to the FFs of the separate gates. Our initial goal is to compute the decay amplitudes Γ_{α} for a sequence of quantum gates, and later on, we will use these results to single out corrections arising from the concatenation alone.

We consider that the control $U_c(t)$ is implemented by concatenating several gates $P_g \equiv U_c(t_g,t_{g-1}), g \in \{1,2,\ldots,G\}$ with $t_0 \equiv 0, t_G \equiv \tau$. Accordingly, we define the cumulative propagators $Q_g = P_g P_{g-1} \cdots P_0$ with $P_0 \equiv 1$ such that the total control operation is given by $Q \equiv Q_G$. Denoting by $Q^{(g-1)}(\bullet) = Q_{g-1}^{\dagger} \bullet Q_{g-1}$ the superoperator transforming to the interaction picture with respect to Q_{g-1} , we can write the interaction picture noise operators at time $t \in (t_{g-1},t_g]$ as

$$\tilde{B}_{\alpha}(t) = \mathcal{Q}^{(g-1)}[\tilde{B}_{\alpha}^{(g)}(t - t_{g-1})],$$
 (9)

where $\tilde{B}_{\alpha}^{(g)}(t)$ are the noise operators in the interaction picture of the gth gate. We obtain the Fourier transform of $\tilde{B}_{\alpha}(t)$ by splitting up the integral into the time intervals $(t_{g-1}, t_g]$,

$$\tilde{B}_{\alpha}(\omega) = \sum_{g=1}^{G} e^{i\omega t_{g-1}} \mathcal{Q}^{(g-1)} [\tilde{B}_{\alpha}^{(g)}(\omega)], \qquad (10)$$

with $\tilde{B}_{\alpha}^{(g)}(\omega)=\int_{0}^{\Delta t_{g}}\mathrm{d}t\mathrm{e}^{\mathrm{i}\omega t}\tilde{B}_{\alpha}^{(g)}(t)$ and $\Delta t_{g}=t_{g}-t_{g-1}$ (cf. Ref. [21]). The terms $\tilde{\mathcal{B}}_{ak}(\omega)=\mathrm{tr}[\tilde{B}_{\alpha}(\omega)\sigma_{k}]$ can now be used to calculate the generalized FFs $F_{\alpha,kl}(\omega)$. Thus, Eq. (10) illustrates that generalized FFs of an entire sequence of gates can be easily calculated if the noise operators $\tilde{B}_{\alpha}^{(g)}(\omega)$ of the single gates have already been computed, for example, by following Ref. [20] or Ref. [28].

Correlation filter functions.—By combining Eqs. (4) and (10), we find leading-order corrections to the quantum process of a sequence of gates that arise solely from the concatenation operation itself and, hence, allow valuable insight into effects relevant for algorithms. We call these corrections, which depend on the positions (g,g') of two gates in a sequence with g=g' corresponding to the regular FF of the gth gate, correlation filter functions (CFFs). We explicitly show this relation for the well-known fidelity FF, but as with regular FFs, one may also derive CFFs for other quantities as linear combinations of generalized CFFs. We use Eq. (8) together with Eqs. (7) and (10) to compute the infidelity $\mathcal{I}=1-\mathcal{F}$ and find that

$$\mathcal{I} =: \sum_{g=1}^{G} \left[\mathcal{I}^{(g)} + \frac{1}{d+1} \sum_{\alpha} \sum_{\substack{g'=1\\g' \neq g}}^{G} \int_{-\infty}^{\infty} \frac{\mathrm{d}\omega}{2\pi} S_{\alpha}(\omega) F_{\alpha}^{(gg')}(\omega) \right], \tag{11}$$

where $\mathcal{I}^{(g)}$ is the infidelity of the gth pulse alone and $F_{\alpha}^{(gg')}(\omega)$ [51] is a FF describing correlation effects between the pulses at positions g and g' in the sequence due to noise source α . By summing over all gates, the regular fidelity FF $F_{\alpha}(\omega) = \sum_{g,g'=1}^G F_{\alpha}^{(gg')}(\omega)$ can be obtained. Unlike $F_{\alpha}(\omega)$, $F_{\alpha}^{(gg')}(\omega)$ is complex valued and not strictly positive (but Hermitian in g and g' so that the sum over all g, g' is real). Moreover, since second order ME terms are traceless, Eq. (11) is exact up to $\mathcal{O}(\xi^4)$.

CFFs can, for example, capture the effect of dynamical error suppression in spin echo experiments, which we can view as a sequence of an idle pulse, a π pulse, and another idle pulse. The regular FFs of each of these individual pulses, that is $F_{\alpha}^{(gg)}(\omega)$ for $g \in \{1, 2, 3\}$, are characterized by a finite value at low frequencies as the idle pulses simply correspond

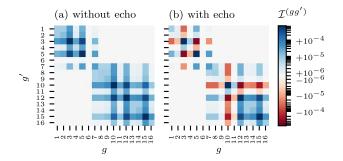


FIG. 1. Correlation infidelities $\mathcal{I}^{(gg')}$ for a four-qubit quantum Fourier transform circuit without (a) and with (b) additional π_x pulses on the fourth qubit. We only consider σ_y noise on the fourth qubit modeled by a 1/f spectral noise density. The indices g, g' = 1, ..., 16 indicate the gates' temporal positions in the circuit. Without the echo pulses, correlations in the noise give rise to significant infidelity contributions for gate pairs up to ten clock cycles apart. Incorporating echoes leads to negative correlation infidelity, given by $\sum_{gg'} \mathcal{I}^{(gg')}$, by more than a factor of 3 for this noise channel.

to free induction decays with FF $\simeq \sin^2(\omega t_g/2)/\omega^2$ [18]. The error cancellation for low frequency dephasing (σ_z) noise then arises mainly from the CFF $F_z^{(1,3)}(\omega) \simeq$ $-\sin^2(\omega\tau_{\rm idle}/2)\exp(i\omega\tau_{\rm idle})/\omega^2$ between the two idle pulses which we may interpret as destructive interference. As a more involved example, consider a quantum Fourier transform [52] on four qubits coupled via nearest neighbor interactions [53]. Using our approach, we investigate the effects of adding spin echos to idling qubits on the total algorithm's fidelity. We apply four π_x pulses on the fourth qubit, two before a controlled phase gate and two afterward [43] and compute the correlation infidelities $\mathcal{I}^{(gg')}=$ $[1/(d+1)]\sum_{\alpha}\int_{-\infty}^{\infty}(\mathrm{d}\omega/2\pi)S_{\alpha}(\omega)F_{\alpha}^{(gg')}(\omega)$ between different pulses [the second term in Eq. (11)]. The results are shown in Fig. 1 for 1/f noise on σ_v on the fourth qubit. Certain pairs of gates have negative correlation infidelities on the order of magnitude of individual gate infidelities, indicating that they cancel errors to a large degree. Indeed, a more than threefold reduction of the total infidelity is observed. Repeating the analysis for white noise reveals that the echo pulses do not change the fidelity significantly.

Conclusion and outlook.—In this work, we have shown how to efficiently obtain process matrices on an arbitrary number of qubits in the presence of correlated classical noise. Many relevant quantities can easily be derived from such a process description, including fidelity measures, measurement statistics, and leakage. In addition, we have introduced the concept of CFFs, which describe corrections when sequences of gates are executed in the presence of noise correlations. As such, CFFs are particularly relevant for testing the notion of independent gates in quantum computing applications, and can be used to calculate

correction terms when this is not the case. CFFs also facilitate the analysis of larger circuits by recycling FFs already computed for individual gates.

We also provide a user-friendly and computationally efficient open source software package [29]. This package, an extension to arbitrary bases, the calculation of several derived quantities, computational efficiency improvements including periodic driving Hamiltonians, and exact results for Gaussian noise based on the cumulant expansion are described in greater detail in Ref. [28]. The latter is particularly relevant for dynamically corrected gates that decouple to lowest order from correlated noise so that second order terms can become dominant [20].

We expect our approach to be useful for analyzing and improving the performance of experimental systems comprising several qubits, for example, by leveraging optimal control approaches [54]. FFs can be more efficient than Monte Carlo methods and directly allow further insight into qualitative effects of different types of noise spectra. Possible applications include the analysis and construction of novel dynamical decoupling sequences, noise spectroscopy protocols, dynamically corrected gates, small algorithms, and quantum error correction protocols. Our results could also facilitate the development of more realistic qubit benchmarking protocols, which fully take noise correlations into account.

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