Reply to "Comment on 'Hermitian stochastic methodology for x-ray superfluorescence' "

Stasis Chuchurka,* Vladislav Sukharnikov, and Nina Rohringer†
Deutsches Elektronen-Synchrotron DESY, 22603 Hamburg, Germany
and Department of Physics, Universität Hamburg, 22761 Hamburg, Germany

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This Reply addresses the Comment by Park, Kim, and Lindberg on our article, "Hermitian stochastic methodology for x-ray superfluorescence" [Phys. Rev. A **109**, 063705 (2024)]. The Comment presents criticism, primarily claiming that our derivations involve "a redefinition of physical variables without a clear rationale." Additionally, it asserts that our methodology closely resembles the stochastic Maxwell-Bloch equations (SMBEs) introduced by Park *et al.* We disagree with these observations. In this Reply, we further elaborate on the rationale behind our derivations, building on the explanation already provided in the original article. Furthermore, we demonstrate that the "redefinition of physical variables" is an example of stochastic gauge freedom, a well-established concept in methodologies based on positive-*P* stochastic equations (PPSEs), which underscores the consistency of our derivations with the PPSE formalism. Additionally, we highlight the fundamental differences between our methodology and the SMBEs.

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I. INTRODUCTION

This Reply addresses the Comment on our recent article [1], where we propose a stochastic framework for simulating x-ray superfluorescence—spontaneous emission from inner-shell atomic transitions amplified in a transiently inverted medium. The article presents a solution to the problem of divergent stochastic trajectories encountered in our earlier attempt to simulate superfluorescence [2]. In their Comment, Park, Kim, and Lindberg raise several points of criticism of our proposed solution, which we contest in this Reply.

The main claim of the Comment is that our derivations involve "a redefinition of physical variables without a clear rationale," allegedly contradicting our original formalism. Specifically, the critique focuses on the derivation of the atomic polarization field $P_s^{(\pm)}(\mathbf{r},\tau)$, a key component in the equations that serves as the source of the electromagnetic field. The Comment separately examines the properties of the deterministic part $P_{s,\mathrm{det}}^{(\pm)}(\mathbf{r},\tau)$ and the stochastic part $P_{s,\mathrm{noise}}^{(\pm)}(\mathbf{r},\tau)$ of the polarization field, claiming inconsistencies between their properties and those of the original formalism in Ref. [2].

We argue that the alleged inconsistencies in the deterministic part $P_{s,\mathrm{det}}^{(\pm)}(\mathbf{r},\tau)$ stem from an apparent misunderstanding of the derivations, an issue that must be addressed for rendering our derivations more accessible to the general reader. The discussion in Sec. II provides sufficient clarification, demonstrating the rigor of the derivations. In Sec. III, we address the alleged inconsistencies regarding the stochastic part $P_{s,\mathrm{noise}}^{(\pm)}(\mathbf{r},\tau)$. We elaborate on the rationale behind our derivations by adding mathematical details. We demonstrate that the so-called "redefinition of physical variables" is an example of stochastic gauge freedom, a well-established concept in methodologies based on positive-*P* stochastic equations (PPSEs) [3–7], thereby underscoring the consistency of our approach with the PPSE formalism.

Finally, in Sec. IV, we highlight the fundamental differences between our methodology and the SMBEs presented in Ref. [8], which cannot be reconciled even within the presented gauge freedom, thereby establishing the independence of the two methods.

II. POLARIZATION FIELD

Park *et al.* compare two expressions for the polarization fields. The first, Eq. (3) of the commented article [1], is the starting point of our derivations:

$$P_s^{(+)}(\mathbf{r},\tau) = n(\mathbf{r}) \sum_{u,l} T_{lu,s}\rho_{ul}(\mathbf{r},\tau) + f_s(\mathbf{r},\tau), \tag{1}$$

$$P_s^{(-)}(\mathbf{r},\tau) = n(\mathbf{r}) \sum_{u,l} T_{ul,s}\rho_{lu}(\mathbf{r},\tau) + g_s(\mathbf{r},\tau) \tag{2}$$

The second, Eq. (10) of Ref. [1], is the result of our derivations, which give an approximation of Eq. (3) in Ref. [1] to spontaneous emission in the perturbative limit:

$$P_s^{(+)}(\mathbf{r},\tau) = n(\mathbf{r}) \sum_{u,l} T_{lu,s}\rho_{ul}(\mathbf{r},\tau) + P_{s,\mathrm{noise}}^{(+)}(\mathbf{r},\tau), \tag{3a}$$

$$P_s^{(-)}(\mathbf{r},\tau) = n(\mathbf{r}) \sum_{u,l} T_{ul,s}\rho_{lu}(\mathbf{r},\tau) + P_{s,\mathrm{noise}}^{(-)}(\mathbf{r},\tau). \tag{3b}$$

We contend that the alleged inconsistencies arise from a misinterpretation of Eq. (3). Without the proper context provided by the derivations in Sec. III of the commented article [1], it might appear that both Eqs. (1), (2) and (3) involve

*Contact author: stasis.chuchurka@desy.de
†Contact author: nina.rohringer@desy.de

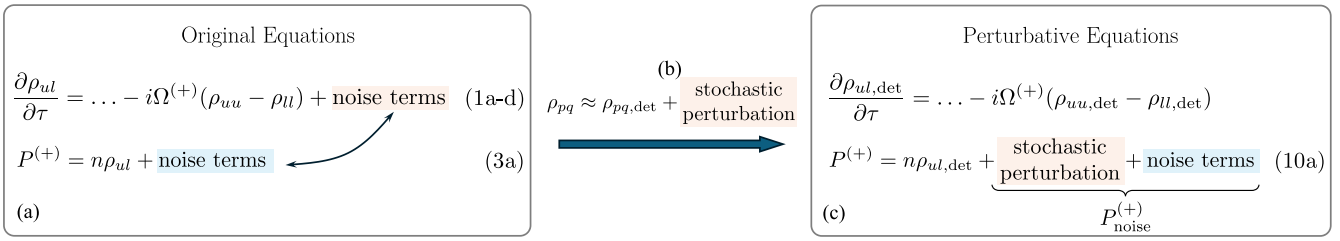

FIG. 1. Schematic illustration of the concept underlying our derivations in Ref. [1]. (a) The original equations include noise in both the atomic variables ρ_{pq} and the full polarization field $P^{(\pm)}$. The goal of the derivations is to reduce the number of stochastic components using reasonable approximations. Assuming that the noise terms generating spontaneous emission have a negligible impact on atomic dynamics, we treat these terms perturbatively. (b) This approach justifies separating ρ_{pq} into a deterministic part and its stochastic perturbation. (c) The deterministic part, $\rho_{pq,\mathrm{det}}$, is governed by the deterministic Bloch equations, while the stochastic perturbation is combined with the original noise in the polarization field $P^{(\pm)}$. Together, these random contributions form a new stochastic component, $P^{(\pm)}_{\mathrm{noise}}$.

identical atomic variables $\rho_{lu}(\mathbf{r},\tau)$, which would indeed lead to "twice the original correlator," as stated by Park *et al.*

However, we emphasize that the atomic variables $\rho_{lu}(\mathbf{r},\tau)$ and $\rho_{ul}(\mathbf{r},\tau)$ in Eqs. (1), (2) and (3) are not identical. Specifically, Eq. (3) incorporates $\rho_{lu,\mathrm{det}}(\mathbf{r},\tau)$ and $\rho_{ul,\mathrm{det}}(\mathbf{r},\tau)$, which were renamed as $\rho_{lu}(\mathbf{r},\tau)$ and $\rho_{ul}(\mathbf{r},\tau)$ for simplicity. This reformulation was explicitly noted in the right-hand column of page 6 of the commented article [1].

The stochastic components of the original atomic variables were transferred to $P^{(-)}_{s,\mathrm{noise}}(\mathbf{r},\tau)$, as illustrated in Fig. 1 and described in its caption. Consequently, the resulting atomic variables $\rho_{lu,\mathrm{det}}(\mathbf{r},\tau)$ and $\rho_{ul,\mathrm{det}}(\mathbf{r},\tau)$ are governed solely by the deterministic Bloch equations and do not include any stochastic components from the initial equations in Sec. II of the commented article. As a result, Eq. (10) of Ref. [1] cannot yield "twice the original correlator," as claimed by Park *et al.*

To avoid potential confusion following the renaming, Sec. IV of the commented article [1] provides further clarification:

> Based on the derivations in Sec. III, we conclude that the Bloch equations (1a)–(1c), *excluding* the noise terms in Eq. (1d), effectively describe the atomic degrees of freedom.

III. PROPERTIES OF THE STOCHASTIC POLARIZATION FIELDS

The other point of criticism raised in the Comment focuses on the properties of the stochastic part of the polarization fields, $P^{(\pm)}_{s,\mathrm{noise}}(\mathbf{r},\tau)$. Park *et al.* challenge the transition from Eqs. (6) and (8) to Eq. (18) of the commented article [1], arguing that the reformulation of the noise terms must remain constrained by their earlier form in Eqs. (6) and (8), as well as by the correlation properties given in Eq. (4) of Ref. [1].

We first recall the definition of the stochastic polarization fields $P^{(+)}_{s,\mathrm{noise}}(\mathbf{r},\tau)$, as given in Eq. (6) of the commented article [1],

$$P^{(+)}_{s,\mathrm{noise}}(\mathbf{r},\tau) \approx f_s(\mathbf{r},\tau) + n(\mathbf{r}) \int_0^\tau d\tau' e^{(\Gamma_u+\Gamma_l)(\tau'-\tau)/2} \times \sum_{s'} \rho^{(\mathrm{up.})}_{ss'}(\mathbf{r},\tau') g^\dagger_{s'}(\mathbf{r},\tau'), \tag{4}$$

with $P^{(-)}_{s,\mathrm{noise}}(\mathbf{r},\tau)$ defined analogously in Eq. (8) of Ref. [1]. The quantity $\rho^{(\mathrm{up.})}_{ss'}(\mathbf{r},\tau')$ is defined in Eq. (7) in Ref. [1]. A schematic but detailed derivation of these expressions is provided in Sec. II of this Reply.

Crucially, the transition to the stochastic polarization fields simplifies the structure of the noise in the model. The four original stochastic terms—$g_s(\mathbf{r},\tau)$, $g^\dagger_s(\mathbf{r},\tau)$, $f_s(\mathbf{r},\tau)$, and $f^\dagger_s(\mathbf{r},\tau)$—are reduced to two: $P^{(\pm)}_{s,\mathrm{noise}}(\mathbf{r},\tau)$. Directly sampling $P^{(\pm)}_{s,\mathrm{noise}}(\mathbf{r},\tau)$ from the original noise terms would result in divergent equations, similar to the ungauged equations in Ref. [2]. In theory, with an infinite number of stochastic realizations, accurate observables can be obtained. In practice, however, only a finite number of trajectories can be generated, which may not fully capture the statistical properties of the system. Diverging trajectories, in particular, disproportionately influence the results, overweighing the contributions of regular trajectories. These divergent realizations cannot be discarded, as they have nonzero measure, and excluding them leads to incorrect results. The transformation proposed in Ref. [1] not only preserves the correct observables in theory but also ensures the absence of divergent trajectories in practice.

A key step in constructing the Hermitian model is the recognition that the only essential requirement for the representation of $P^{(\pm)}_{s,\mathrm{noise}}(\mathbf{r},\tau)$ is the correlators specified in Eq. (9) of Ref. [1]. Indeed, the stochastic methodology involves generating a sufficiently large sample of stochastic realizations, which are then used to calculate expectation values. These averages depend not on the specific realizations of the random components but on correlators of the noise terms, involved in the equations of motion. As long as the correlation properties of the random components in the equations—specifically $P^{(\pm)}_{s,\mathrm{noise}}(\mathbf{r},\tau)$—are preserved, their form can vary. From Eqs. (6) and (8) of Ref. [1] for the stochastic polarization fields, we can obtain their correlation properties, which are given in Eq. (9) of the commented article [1]. These follow directly from the original correlation properties provided in Eq. (4) of Ref. [1].

In this Reply, we strengthen the argument that only the correlation properties in Eq. (9) of Ref. [1] matter, while the explicit form of the noise terms can vary, showing the invariance of the characteristic functional that generates all the relevant averages.

For clarity, we consider a one-dimensional case, two-level atoms, and ignore all but one polarization component of the field. In this case, the field variables $\Omega^{(\pm)}(z,\tau)$ depend only

on the propagation coordinate z and retarded time τ. All the essential field expectation values can be stored in the characteristic (generative) functional that we define as follows,

$$\chi(z,\{\lambda\}) = \langle X(z,\{\lambda\})\rangle,$$

where the functional $X(z,\{\lambda\})$ is given by

$$X(z,\{\lambda\}) = \exp\left\{\int \lambda^{(+)}(\tau)\Omega^{(+)}(z,\tau)d\tau + \int \lambda^{(-)}(\tau)\Omega^{(-)}(z,\tau)d\tau\right\}.$$

The field observables are extracted by taking functional derivatives with respect to $\lambda^{(+)}(\tau)$ and $\lambda^{(-)}(\tau)$. For example, the first-order field correlation function can be obtained by

$$\langle\Omega^{(+)}(z,\tau)\Omega^{(-)}(z,\tau')\rangle = \left.\frac{\delta^2\chi(z,\{\lambda\})}{\delta\lambda^{(+)}(\tau)\delta\lambda^{(-)}(\tau')}\right|_{\lambda=0}.$$

Note that $\chi(z,\{\lambda\})$ does not involve atomic variables, as these are secondary and can be fully determined from the properties of the field variables.

We further present derivations following the same approach as in Appendix A of Ref. [9]. Since the field variables are only known in differential form, we do not have a closed analytic expression for the characteristic functional. Therefore, we adopt an inductive approach and we instead show that the derivative of the characteristic functional with respect to z remains independent of the explicit form of the noise terms.

The key distinction between the derivations in this Reply and those in Ref. [9] lies in the primary dynamic objects: In the compact system, these are atomic variables, whereas, in our case of an extended system, they are field variables. The primary role of the field variables defines the most natural parametrization for the characteristic functional. It must be parametrized by z, as the equations for the field variables (17) in the commented article [1] feature the derivative with respect to z:

$$\frac{\partial}{\partial z}\Omega^{(+)}(z,\tau) = i\frac{3}{8\pi}\lambda_0^2\Gamma_{\rm rad}[n\rho_{ul}(z,\tau) + P^{(+)}_{\rm noise}(z,\tau)], \quad (5)$$

$$\frac{\partial}{\partial z}\Omega^{(-)}(z,\tau) = -i\frac{3}{8\pi}\lambda_0^2\Gamma_{\rm rad}[n\rho_{lu}(z,\tau) + P^{(-)}_{\rm noise}(z,\tau)]. \quad (6)$$

According to Eq. (9) of Ref. [1], the noise terms, adopted for the one-dimensional case, have the following correlation properties:

$$\langle P^{(+)}_{\rm noise}(z,\tau)P^{(+)}_{\rm noise}(z',\tau')\rangle = \sigma^{(+)}(z,\tau,\tau')\delta(z-z') = 0, \quad (7)$$

$$\langle P^{(-)}_{\rm noise}(z,\tau)P^{(-)}_{\rm noise}(z',\tau')\rangle = \sigma^{(-)}(z,\tau,\tau')\delta(z-z') = 0, \quad (8)$$

$$\begin{aligned}\langle P^{(+)}_{\rm noise}(z,\tau)P^{(-)}_{\rm noise}(z',\tau')\rangle &= \sigma(z,\tau,\tau')\delta(z-z')\\ &= n(z)\,e^{-\Gamma|\tau-\tau'|/2}\rho^{(\rm up)}(z,\min[\tau,\tau'])\,\delta(z-z'),\end{aligned} \quad (9)$$

where $\rho^{(\rm up)}(\mathbf{r},\tau)$ is given by Eq. (14) of Ref. [1]:

$$\rho^{(\rm up)}(z,\tau) = \rho_{uu}(z,\tau) - \rho_{ul}(z,\tau)\rho_{lu}(z,\tau).$$

The correlators in Eq. (9) of Ref. [1] describe a colored process with respect to the retarded time, featuring a memory timescale of Γ^{-1}, which is determined by the decay rate of the involved atomic transition. Here, we adopt a more general notation with $\sigma^{(+)}(z,\tau,\tau')$, $\sigma^{(-)}(z,\tau,\tau')$, and $\sigma(z,\tau,\tau')$ to emphasize that only these three correlators are significant and must be preserved (assuming the mean of the noise terms remains zero). The specific method by which the correlators are obtained is irrelevant.

Using Itô's interpretation of stochastic differential equations (17) of Ref. [1], we apply Itô's rule, yielding

$$\begin{aligned}\frac{d\chi(z,\{\lambda\})}{dz} = \left\langle\frac{dX(z,\{\lambda\})}{dz}\right\rangle &= i\frac{3}{8\pi}\lambda_0^2\Gamma_{\rm rad}n\left\langle\int d\tau\left[\rho_{ul}(z,\tau)\lambda^{(+)}(\tau) - \rho_{lu}(z,\tau)\lambda^{(-)}(\tau)\right]X(z,\{\lambda\})\right\rangle\\ &+\left[\frac{3}{8\pi}\lambda_0^2\Gamma_{\rm rad}\right]^2\left\langle\int d\tau d\tau'\,\sigma(z,\tau,\tau')\lambda^{(+)}(\tau)\lambda^{(-)}(\tau')X(z,\{\lambda\})\right\rangle\\ &+\frac{1}{2}\left[\frac{3}{8\pi}\lambda_0^2\Gamma_{\rm rad}\right]^2\left\langle\int d\tau d\tau'\,\sigma^{(+)}(z,\tau,\tau')\lambda^{(+)}(\tau)\lambda^{(+)}(\tau')X(z,\{\lambda\})\right\rangle\\ &+\frac{1}{2}\left[\frac{3}{8\pi}\lambda_0^2\Gamma_{\rm rad}\right]^2\left\langle\int d\tau d\tau'\,\sigma^{(-)}(z,\tau,\tau')\lambda^{(-)}(\tau)\lambda^{(-)}(\tau')X(z,\{\lambda\})\right\rangle.\end{aligned}$$

The resulting expression demonstrates that the derivative is influenced solely by the structure of the deterministic part and the correlators $\sigma^{(+)}(z,\tau,\tau')$, $\sigma^{(-)}(z,\tau,\tau')$ and $\sigma(z,\tau,\tau')$. Since both remain unchanged under a "redefinition of physical variables," this justifies adopting any specific form for the stochastic polarization fields as long as the relevant correlators are preserved.

One possible representation, provided in Eqs. (11)–(13) of the commented article [1], introduces new noise terms $F_s(\mathbf{r},\tau)$ and auxiliary functions $\xi_{ss'}(\mathbf{r},\tau)$. This representation ensures that the physical variables remain Hermitian, which guarantees stable stochastic realizations.

The choice to impose Hermiticity on the stochastic variables enables each individual stochastic trajectory to be interpreted as a physically meaningful experimental realization. Specifically, all realizations exhibit "realistic" properties—such as real and positive photon numbers, and Hermitian atomic density matrices—while their statistical averages yield the correct expectation values and correlation functions.

As the derivations are identical to those in Appendix A of Ref. [9], the described freedom can be viewed as an example of the stochastic gauge freedom widely used in methodologies based on positive-P stochastic equations [3–7].

IV. COMPARISON OF METHODS

The Comment frequently mentions the resemblance between our approaches. However, we argue that establishing such a connection requires a more rigorous justification than merely pointing to symbolic or visual similarities, as done in Eq. (4) of the Comment.

The similarity between the methods lies solely in the attempt to use random numbers to describe spontaneous emission—an idea that is not new and has been widely utilized. For instance, the approach in Ref. [10], which we employed for comparison in our work, is a well-established example.

Stochastic methods differ in their models for random numbers, their correlation properties, and their roles in the equations. Here, we aim to demonstrate that our method is fundamentally distinct from the approach presented by the Comment authors in Ref. [8]. To demonstrate this distinction, it is sufficient to examine the differences in the stochastic components of the equations.

Equation (4) of the Comment postulates the following mapping between our noise terms, $P^{(\pm)}_{s,\mathrm{noise}}$, and the noise terms ξ from Ref. [8]:

$$P^{(+)}_{s,\mathrm{noise}} \leftrightarrow \xi^*, \quad P^{(-)}_{s,\mathrm{noise}} \leftrightarrow \xi. \tag{10}$$

This suggests a complete correspondence between the objects. However, as we will demonstrate, these objects fundamentally differ in their mathematical formulations.

Our noise terms, simplified for the case of two-level atoms with a single field polarization component, have the correlation properties:

$$\langle P^{(+)}_{\mathrm{noise}}(\mathbf{r},\tau) P^{(-)}_{\mathrm{noise}}(\mathbf{r}',\tau')\rangle = n(\mathbf{r}) e^{-\Gamma|\tau-\tau'|/2} \rho^{(\mathrm{up})}(\mathbf{r}, \min[\tau,\tau'])\delta(\mathbf{r}-\mathbf{r}'), \tag{11}$$

where $\rho^{(\mathrm{up})}(\mathbf{r},\tau)$ is given by Eq. (14) of Ref. [1]:

$$\rho^{(\mathrm{up})}(\mathbf{r},\tau) = \rho_{uu}(\mathbf{r},\tau) - \rho_{ul}(\mathbf{r},\tau)\rho_{lu}(\mathbf{r},\tau).$$

The decay rate related to the transition is denoted by Γ. The correlator in Eq. (11) defines a colored Ornstein-Uhlenbeck process, which includes the memory effect on the correlation timescale of Γ^{-1}, which is crucial for accurate reproduction of spectral properties of the emission.

Notably, the correlator, that can be directly mapped to Eq. (11), was also derived in one of our preprints [see Ref. [11] from 1 Mar 2023, Eq. (42)], prior to the appearance of the preprint of Park *et al.* in Ref. [8].

Regarding the quantities ξ and ξ^*, referring to Eq. (28) of Ref. [8], we find that these are random numbers defined as

$$\xi_{(n)} = \sqrt{\rho_{uu(n)} - |\rho_{lu(n)}|^2}\, e^{i\Phi_{(n)}},$$

where index n labels time points, and $\Phi_{(n)}$ are independent random phases. The random numbers $\xi_{(n)}$ have the following correlation properties,

$$\langle \xi_{(n)}\, \xi^*_{(m)}\rangle = \delta_{nm}|\rho_{uu(n)} - |\rho_{lu(n)}|^2|, \tag{12}$$

indicating that $\xi_{(n)}$ and $\xi^*_{(m)}$ are statistically independent for distinct time points $n \neq m$. In contrast, our noise terms incorporate memory effects over a timescale determined by Γ^{-1}.

Additionally, our stochastic terms have a well-defined mathematical meaning in the limit of infinitely small propagation time steps. In contrast, the methodology proposed by Park *et al.* in Ref. [8] is restricted to finite, discrete time steps.

Furthermore, our noise terms are found as a solution to stochastic differential equation in Eq. (11) of Ref. [1], and appear solely in the field equation as a fluctuating source (see Sec. IV of Ref. [1]). As for the random numbers $\xi_{(n)}$, they enter all equations of motion through variables with hats [see Eqs. (27)–(31) of Ref. [8]).

As a result, the claimed correspondence (10) between the colored Ornstein-Uhlenbeck process in Eq. (11) and the random numbers without memory effects in Eq. (12) lacks any valid justification. Our stochastic polarization fields cannot be reduced to the random contributions ξ and ξ^*, even within the gauge freedom discussed earlier. This is because the gauge freedom is designed to preserve the correlator—a fundamental property of the noise terms that differs between the compared frameworks.

V. DISCUSSION AND CONCLUSION

We have clarified the rationale behind the derivations in our original article, highlighting the consistency of our approach with the positive-P stochastic equation (PPSE) formalism, particularly the concept of stochastic gauge freedom.

We also emphasize that the original derivations, as well as the discussion presented in this Reply, can be extended to a more general setting, which will be explored in future publications. In particular, the framework allows for arbitrary level lifetimes and detunings. Furthermore, while Ref. [1] focused on pumping via photoionization, described by the nonunitary part of the Bloch equations, the method can also be generalized to resonant pumping scenarios, which involve the unitary terms of the Bloch equations.

Additionally, we have shown that the methodology proposed in our work is fundamentally distinct from the SMBEs. The noise terms in our model, which incorporate memory effects and are derived from stochastic differential equations, cannot be reconciled with the random number representations used in the SMBEs, which have different correlation properties.

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